



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 06:28 am BST

PDB ID : 5GUW  
Title : Complex of Cytochrome cd1 Nitrite Reductase and Nitric Oxide Reductase in Denitrification of *Pseudomonas aeruginosa*  
Authors : Terasaka, E.; Sugimoto, H.; Shiro, Y.; Tosha, T.  
Deposited on : 2016-08-31  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

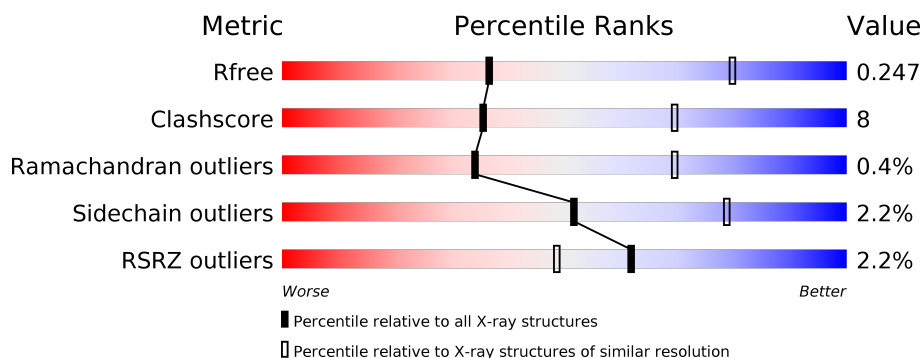
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	146	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div></div> </div> <div></div> </div>
1	C	146	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div></div> </div> <div></div> </div>
2	B	465	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div></div> </div> <div></div> </div>
2	D	465	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div></div> </div> <div></div> </div>
3	M	568	<div> <div></div> <div> <div></div> <div>77%</div> <div>17%</div> <div></div> </div> <div></div> </div>
3	N	568	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div></div> </div> <div></div> </div>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18387 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nitric oxide reductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1123	720	195	202	6			
1	C	142	Total	C	N	O	S	0	0	0
			1123	720	195	202	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	LYS	ASN	conflict	UNP Q59646
C	100	LYS	ASN	conflict	UNP Q59646

- Molecule 2 is a protein called Nitric oxide reductase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	449	Total	C	N	O	S	0	0	0
			3576	2416	563	572	25			
2	D	449	Total	C	N	O	S	0	0	0
			3576	2416	563	572	25			

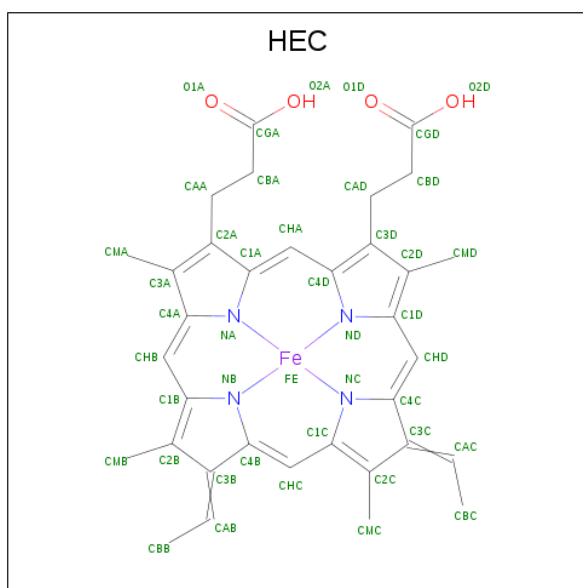
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ARG	deletion	UNP Q59647
D	?	-	ARG	deletion	UNP Q59647

- Molecule 3 is a protein called Nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	538	Total	C	N	O	S	0	0	0
			4203	2665	733	793	12			
3	N	538	Total	C	N	O	S	0	0	0
			4203	2665	733	793	12			

- Molecule 4 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).

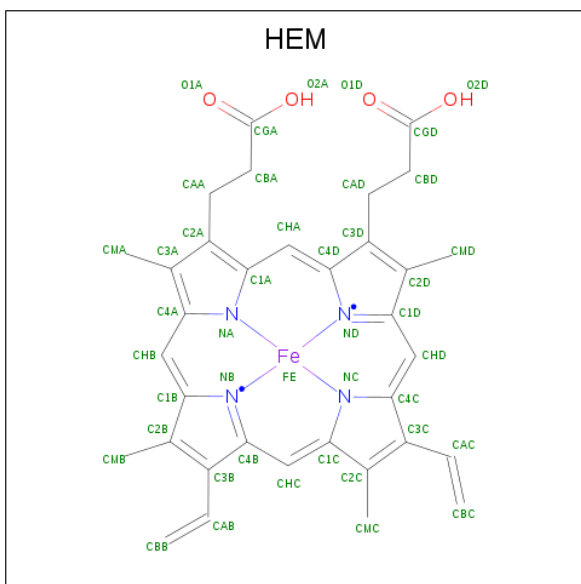


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	M	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	N	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca		
			1	1	0	0
5	C	1	Total	Ca		
			1	1	0	0

- Molecule 6 is decyl 4-O-alpha-D-glucopyranosyl-1-thio-beta-D-glucopyranoside (three-letter code: 10M) (formula:  $C_{22}H_{42}O_{10}S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
7	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
7	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
7	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	

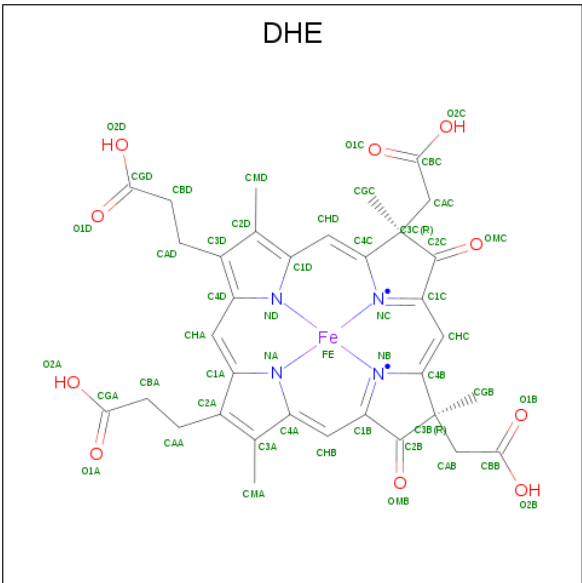
- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Fe		
			1	1	0	0
8	D	1	Total	Fe		
			1	1	0	0

- Molecule 9 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	O		
			1	1	0	0
9	D	1	Total	O		
			1	1	0	0

- Molecule 10 is HEME D (three-letter code: DHE) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	M	1	Total	C	Fe	N	O	0	0
			49	34	1	4	10		
10	N	1	Total	C	Fe	N	O	0	0
			49	34	1	4	10		

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	N	1	Total	Cl	0	0
			1	1		
11	M	1	Total	Cl	0	0
			1	1		

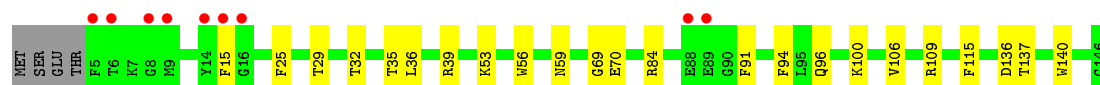
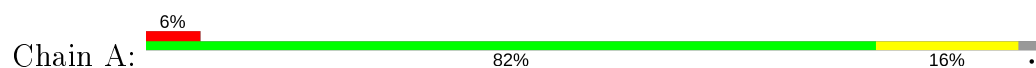
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	3	Total	O	0	0
			3	3		
12	B	11	Total	O	0	0
			11	11		
12	C	6	Total	O	0	0
			6	6		
12	D	6	Total	O	0	0
			6	6		
12	M	5	Total	O	0	0
			5	5		
12	N	3	Total	O	0	0
			3	3		

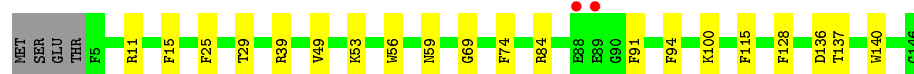
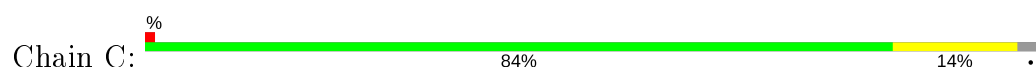
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

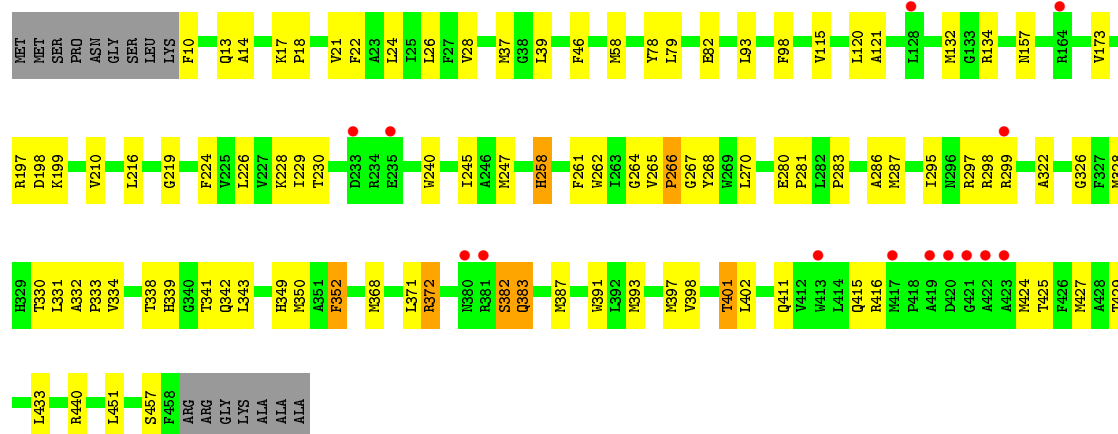
#### • Molecule 1: Nitric oxide reductase subunit C



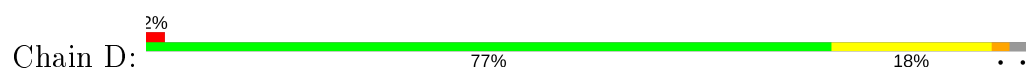
#### • Molecule 1: Nitric oxide reductase subunit C



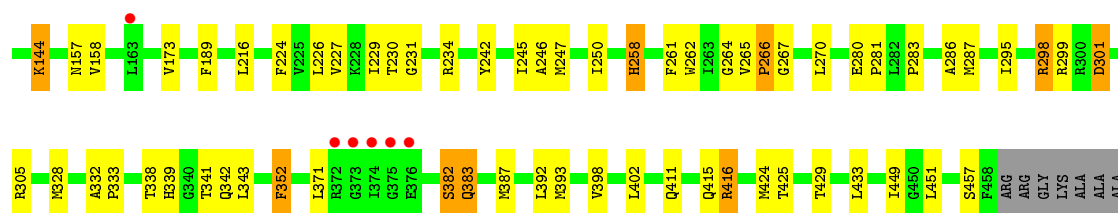
#### • Molecule 2: Nitric oxide reductase subunit B



#### • Molecule 2: Nitric oxide reductase subunit B

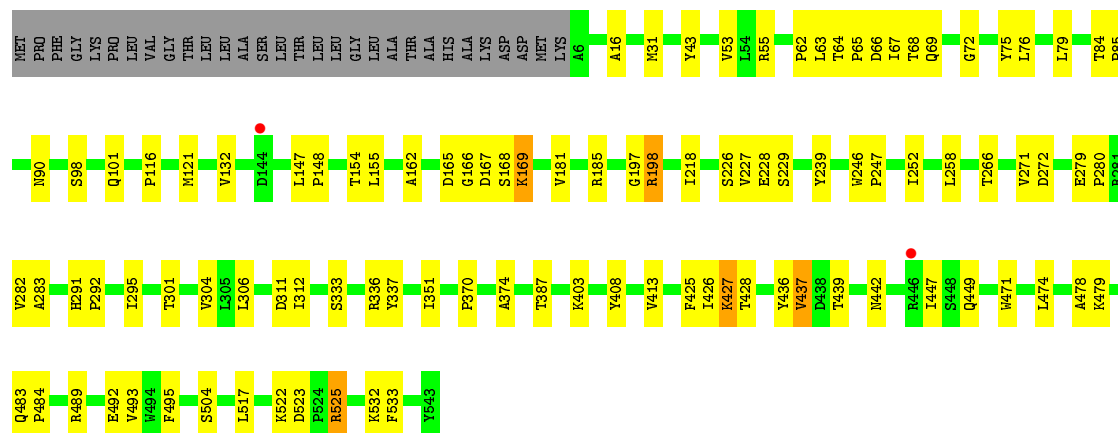






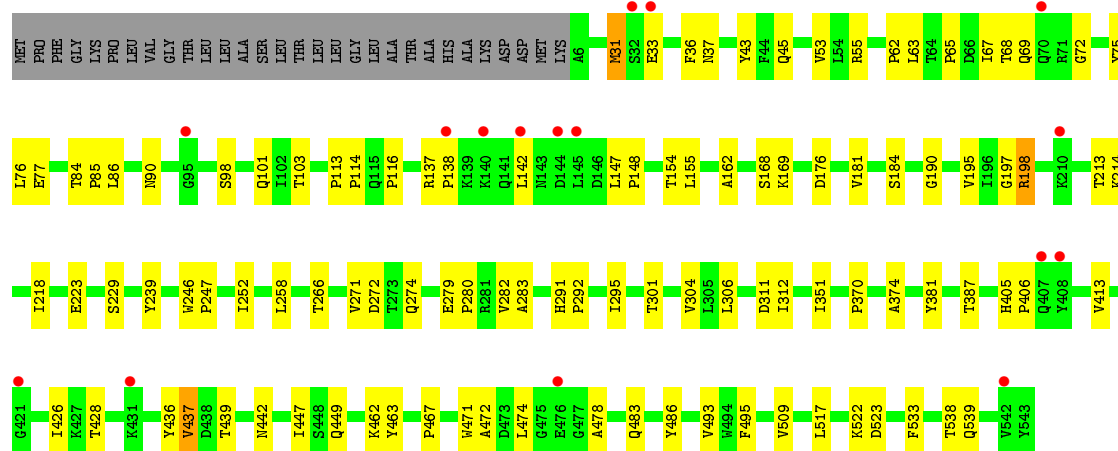
• Molecule 3: Nitrite reductase

Chain M: 77% 17% • 5%



• Molecule 3: Nitrite reductase

Chain N: 3% 76% 18% • 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.87Å 128.61Å 127.81Å 90.00° 106.83° 90.00°	Depositor
Resolution (Å)	49.48 – 3.20 49.43 – 3.20	Depositor EDS
% Data completeness (in resolution range)	87.7 (49.48-3.20) 87.5 (49.43-3.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 3.19Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.210 , 0.254 0.208 , 0.247	Depositor DCC
$R_{free}$ test set	2551 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.2	Xtrriage
Anisotropy	0.120	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	18387	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6858e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 10M, DHE, CL, O, FE, HEC, HEM, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.41	0/1153	0.61	0/1559
1	C	0.45	0/1153	0.62	0/1559
2	B	0.41	0/3693	0.61	0/5039
2	D	0.45	0/3693	0.62	0/5039
3	M	0.43	0/4308	0.65	0/5854
3	N	0.40	0/4308	0.65	0/5854
All	All	0.42	0/18308	0.63	0/24904

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1123	0	1091	21	0
1	C	1123	0	1091	15	0
2	B	3576	0	3619	70	1
2	D	3576	0	3619	60	1
3	M	4203	0	4158	65	0
3	N	4203	0	4158	68	0
4	A	43	0	31	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	43	0	32	5	0
4	M	43	0	31	4	0
4	N	43	0	32	4	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	33	0	42	0	0
6	C	33	0	42	0	0
6	D	33	0	42	0	0
7	B	86	0	60	8	0
7	D	86	0	60	6	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	M	49	0	28	7	0
10	N	49	0	28	3	0
11	M	1	0	0	0	0
11	N	1	0	0	0	0
12	A	3	0	0	0	0
12	B	11	0	0	1	0
12	C	6	0	0	0	0
12	D	6	0	0	0	0
12	M	5	0	0	0	0
12	N	3	0	0	0	0
All	All	18387	0	18164	295	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (295) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:16:ALA:HB3	3:N:223:GLU:HG3	1.56	0.87
3:M:169:LYS:NZ	3:M:492:GLU:OE2	2.10	0.83
3:M:165:ASP:HB3	3:M:168:SER:HB3	1.61	0.80
2:B:393:MET:HE1	2:B:451:LEU:HD13	1.64	0.79
1:A:84:ARG:NH1	4:A:201:HEC:O2A	2.16	0.78
3:N:471:TRP:CE3	3:N:517:LEU:HB3	2.19	0.78
2:D:393:MET:HE1	2:D:451:LEU:HD13	1.64	0.78
2:D:104:ALA:O	2:D:108:THR:HG22	1.85	0.76
3:M:336:ARG:NH1	3:M:337:TYR:CZ	2.54	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:176:ASP:O	3:N:214:LYS:HE2	1.87	0.75
2:B:350:MET:HB2	2:B:401:THR:HG21	1.70	0.74
2:B:13:GLN:NE2	2:B:78:TYR:O	2.22	0.71
7:B:801:HEM:HBB2	7:B:801:HEM:HHC	1.71	0.71
3:M:98:SER:OG	3:M:101:GLN:HG3	1.91	0.70
3:M:147:LEU:HB2	3:M:148:PRO:HD3	1.73	0.69
2:B:372:ARG:HG2	2:B:372:ARG:HH11	1.58	0.69
3:N:198:ARG:NH2	10:N:602:DHE:O2B	2.26	0.69
1:A:59:ASN:HB2	4:A:201:HEC:HBB1	1.75	0.69
3:N:147:LEU:HB2	3:N:148:PRO:HD3	1.73	0.68
4:M:601:HEC:HMB1	4:M:601:HEC:HBB3	1.78	0.66
2:D:246:ALA:O	2:D:250:ILE:HD12	1.96	0.65
3:N:169:LYS:HE3	3:N:509:VAL:HG21	1.78	0.65
7:D:801:HEM:HBB2	7:D:801:HEM:HHC	1.79	0.64
2:B:397:MET:O	2:B:401:THR:HG23	1.98	0.63
2:D:411:GLN:HB2	2:D:433:LEU:HD21	1.80	0.63
1:A:70:GLU:OE1	2:B:199:LYS:HD3	1.98	0.63
2:B:411:GLN:HB2	2:B:433:LEU:HD21	1.80	0.63
4:A:201:HEC:HAD1	2:B:427:MET:CE	2.29	0.62
1:A:115:PHE:HZ	4:A:201:HEC:HMC2	1.64	0.62
2:B:425:THR:O	2:B:429:THR:HG23	2.01	0.61
3:M:166:GLY:O	3:M:169:LYS:NZ	2.20	0.61
3:M:90:ASN:O	3:M:90:ASN:OD1	2.18	0.61
2:D:352:PHE:HB3	7:D:801:HEM:CBC	2.31	0.60
3:N:381:TYR:CD1	3:N:413:VAL:CG2	2.85	0.59
3:M:55:ARG:HB3	3:M:63:LEU:HB2	1.84	0.59
3:N:190:GLY:CA	3:N:539:GLN:OE1	2.50	0.59
2:B:352:PHE:HB3	7:B:801:HEM:CBC	2.33	0.59
2:D:425:THR:O	2:D:429:THR:HG23	2.02	0.59
4:A:201:HEC:HAD1	2:B:427:MET:HE2	1.84	0.59
3:N:493:VAL:HG12	3:N:495:PHE:CE1	2.38	0.58
1:A:36:LEU:HD23	2:B:197:ARG:CG	2.33	0.58
1:A:32:THR:HG1	2:B:268:TYR:HH	1.44	0.58
2:D:229:ILE:HG13	2:D:230:THR:HG23	1.85	0.58
3:M:336:ARG:NH1	3:M:337:TYR:OH	2.36	0.58
2:D:93:LEU:HA	2:D:96:ILE:HG22	1.86	0.58
3:M:425:PHE:HE1	10:M:602:DHE:HBD1	1.68	0.57
4:N:601:HEC:HMB1	4:N:601:HEC:HBB3	1.87	0.57
3:M:155:LEU:HD11	3:M:162:ALA:HB2	1.86	0.57
3:M:311:ASP:C	3:M:311:ASP:OD1	2.43	0.57
3:N:155:LEU:HD11	3:N:162:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:381:TYR:CD1	3:N:413:VAL:HG22	2.39	0.57
3:N:55:ARG:HB3	3:N:63:LEU:HB2	1.87	0.57
2:B:229:ILE:HG13	2:B:230:THR:HG23	1.87	0.57
3:M:523:ASP:OD1	3:M:525:ARG:HG2	2.05	0.56
2:B:267:GLY:HA2	2:B:270:LEU:HD13	1.86	0.56
3:M:408:TYR:HB3	3:M:413:VAL:HG11	1.87	0.56
3:N:311:ASP:OD1	3:N:311:ASP:C	2.44	0.56
3:M:167:ASP:OD1	3:M:489:ARG:NH2	2.39	0.56
7:D:801:HEM:HBC2	7:D:801:HEM:HHH	1.86	0.56
3:M:336:ARG:NH1	3:M:337:TYR:CE1	2.74	0.56
3:M:181:VAL:HA	3:M:197:GLY:HA2	1.88	0.55
3:M:439:THR:HG21	3:M:447:ILE:CG2	2.36	0.55
2:B:415:GLN:HB2	2:B:429:THR:HG21	1.88	0.55
2:D:17:LYS:O	2:D:21:VAL:HG23	2.06	0.55
2:B:17:LYS:O	2:B:21:VAL:HG23	2.07	0.55
2:D:415:GLN:HB2	2:D:429:THR:HG21	1.88	0.55
2:D:258:HIS:CE1	7:D:802:HEM:CHD	2.90	0.55
3:N:181:VAL:HA	3:N:197:GLY:HA2	1.89	0.55
3:M:198:ARG:NH2	10:M:602:DHE:O2B	2.40	0.55
1:C:136:ASP:O	2:D:264:GLY:HA2	2.07	0.54
4:A:201:HEC:HMC1	4:A:201:HEC:HBC3	1.89	0.54
2:B:18:PRO:HB2	2:B:98:PHE:CE2	2.42	0.54
2:D:216:LEU:HD11	2:D:245:ILE:HG23	1.89	0.54
3:M:439:THR:HG22	3:M:442:ASN:HB2	1.90	0.54
3:M:185:ARG:HD2	3:M:228:GLU:HA	1.89	0.54
3:N:439:THR:HG21	3:N:447:ILE:CG2	2.37	0.54
3:N:86:LEU:HD12	4:N:601:HEC:O1D	2.08	0.54
2:D:224:PHE:O	2:D:227:VAL:HG12	2.08	0.54
2:B:216:LEU:HD11	2:B:245:ILE:HG23	1.90	0.54
3:N:472:ALA:CB	3:N:474:LEU:HD11	2.38	0.54
2:B:368:MET:O	2:B:372:ARG:HD3	2.08	0.53
3:N:252:ILE:CG2	3:N:312:ILE:HD11	2.38	0.53
3:N:426:ILE:HG13	3:N:437:VAL:HG12	1.90	0.53
10:M:602:DHE:O2C	10:M:602:DHE:C2C	2.56	0.53
3:M:427:LYS:HD3	3:M:484:PRO:O	2.09	0.53
3:N:169:LYS:CE	3:N:509:VAL:HG21	2.38	0.53
3:M:279:GLU:N	3:M:280:PRO:HD3	2.23	0.53
3:M:493:VAL:HG12	3:M:495:PHE:CE1	2.44	0.53
3:M:226:SER:OG	10:M:602:DHE:O2A	2.26	0.53
2:D:14:ALA:HA	2:D:371:LEU:HD22	1.91	0.53
2:D:13:GLN:NE2	2:D:78:TYR:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:252:ILE:CG2	3:M:312:ILE:HD11	2.39	0.53
3:N:533:PHE:HZ	10:N:602:DHE:HAD1	1.74	0.53
2:B:352:PHE:HB3	7:B:801:HEM:HBC2	1.91	0.53
2:D:267:GLY:HA2	2:D:270:LEU:HD13	1.90	0.53
1:A:36:LEU:HD23	2:B:197:ARG:HG3	1.91	0.53
3:M:43:TYR:OH	3:M:55:ARG:HG2	2.09	0.53
3:N:43:TYR:OH	3:N:55:ARG:HG2	2.09	0.53
3:N:67:ILE:HG22	3:N:68:THR:N	2.24	0.53
1:A:136:ASP:O	2:B:264:GLY:HA2	2.09	0.52
3:M:185:ARG:HD2	3:M:227:VAL:O	2.08	0.52
3:M:426:ILE:HG13	3:M:437:VAL:HG12	1.89	0.52
3:N:381:TYR:CE1	3:N:413:VAL:HG22	2.44	0.52
2:D:383:GLN:O	2:D:387:MET:HG3	2.10	0.52
3:N:184:SER:HB3	3:N:195:VAL:HG12	1.91	0.52
4:M:601:HEC:HMB1	4:M:601:HEC:CBB	2.39	0.52
2:B:14:ALA:HA	2:B:371:LEU:HD22	1.91	0.52
3:N:280:PRO:HB3	3:N:301:THR:HG23	1.92	0.52
2:B:266:PRO:CB	2:B:268:TYR:CE2	2.93	0.52
1:A:137:THR:OG1	2:B:262:TRP:O	2.28	0.52
3:M:449:GLN:NE2	3:M:478:ALA:O	2.43	0.52
3:N:439:THR:HG22	3:N:442:ASN:HB2	1.92	0.52
1:C:84:ARG:NH1	4:C:201:HEC:O2A	2.42	0.51
2:B:383:GLN:O	2:B:387:MET:HG3	2.10	0.51
3:N:279:GLU:N	3:N:280:PRO:HD3	2.25	0.51
3:M:425:PHE:CE1	10:M:602:DHE:HBD1	2.45	0.51
3:M:280:PRO:HB3	3:M:301:THR:HG23	1.93	0.51
2:B:115:VAL:HG13	2:B:120:LEU:HB2	1.93	0.51
3:M:523:ASP:OD1	3:M:525:ARG:CG	2.58	0.51
3:N:190:GLY:HA2	3:N:539:GLN:OE1	2.11	0.51
1:A:69:GLY:HA3	2:B:339:HIS:CD2	2.46	0.51
2:B:39:LEU:HD23	2:B:46:PHE:CE2	2.46	0.51
3:N:462:LYS:HG2	3:N:463:TYR:O	2.11	0.50
2:B:121:ALA:HA	2:B:132:MET:CE	2.41	0.50
2:B:424:MET:HB3	2:B:429:THR:HG22	1.94	0.50
3:N:374:ALA:HB1	3:N:428:THR:HG22	1.93	0.50
2:D:19:TYR:CE2	2:D:77:TYR:CE2	3.00	0.50
3:M:64:THR:OG1	3:M:66:ASP:OD1	2.18	0.50
2:D:18:PRO:HB2	2:D:98:PHE:CE2	2.47	0.50
1:A:25:PHE:O	1:A:29:THR:HG23	2.13	0.49
3:N:472:ALA:HB3	3:N:474:LEU:HD11	1.95	0.49
3:N:84:THR:HB	3:N:85:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:601:HEC:HMC1	4:N:601:HEC:HBC3	1.95	0.49
3:N:53:VAL:HG11	3:N:116:PRO:CG	2.42	0.49
2:B:93:LEU:HD23	2:B:157:ASN:HB2	1.95	0.48
2:D:121:ALA:HA	2:D:132:MET:CE	2.42	0.48
1:C:69:GLY:HA3	2:D:339:HIS:CD2	2.48	0.48
2:D:247:MET:CE	2:D:286:ALA:HB2	2.43	0.48
3:N:154:THR:HG21	3:N:181:VAL:O	2.12	0.48
2:D:280:GLU:N	2:D:281:PRO:HD2	2.29	0.48
2:B:82:GLU:OE1	2:B:228:LYS:HE3	2.13	0.48
3:N:304:VAL:HG21	3:N:351:ILE:HD11	1.95	0.48
2:D:258:HIS:HA	2:D:261:PHE:CZ	2.48	0.48
2:B:247:MET:CE	2:B:286:ALA:HB2	2.43	0.48
2:D:173:VAL:HG11	2:D:245:ILE:HD11	1.94	0.48
2:D:424:MET:HB3	2:D:429:THR:HG22	1.94	0.48
1:C:137:THR:OG1	2:D:262:TRP:O	2.32	0.48
3:M:154:THR:HG21	3:M:181:VAL:O	2.13	0.48
3:M:295:ILE:HG12	3:M:306:LEU:HD22	1.96	0.48
3:N:486:TYR:CE1	3:N:493:VAL:HG22	2.49	0.48
1:C:25:PHE:O	1:C:29:THR:HG23	2.13	0.48
3:M:53:VAL:HG11	3:M:116:PRO:CG	2.44	0.48
1:A:96:GLN:O	1:A:100:LYS:HG2	2.14	0.47
2:D:339:HIS:O	2:D:416:ARG:NH1	2.34	0.47
3:N:295:ILE:HG12	3:N:306:LEU:HD22	1.96	0.47
2:B:265:VAL:HB	2:B:266:PRO:HD2	1.96	0.47
2:D:88:LEU:HD11	2:D:158:VAL:HG12	1.95	0.47
2:B:398:VAL:O	2:B:402:LEU:HG	2.15	0.47
2:B:280:GLU:N	2:B:281:PRO:HD2	2.30	0.47
2:B:121:ALA:HA	2:B:132:MET:HE1	1.96	0.47
1:C:59:ASN:HB2	4:C:201:HEC:HBB1	1.95	0.47
2:B:258:HIS:HA	2:B:261:PHE:CZ	2.49	0.47
2:D:341:THR:HG22	2:D:343:LEU:H	1.79	0.47
2:B:341:THR:HG22	2:B:343:LEU:H	1.80	0.47
4:C:201:HEC:HBC3	4:C:201:HEC:HMC1	1.96	0.47
2:B:173:VAL:HG11	2:B:245:ILE:HD11	1.97	0.46
3:M:67:ILE:HG22	3:M:68:THR:N	2.29	0.46
3:M:304:VAL:HG21	3:M:351:ILE:HD11	1.96	0.46
3:N:246:TRP:HA	3:N:247:PRO:C	2.36	0.46
2:B:79:LEU:HB2	2:B:224:PHE:CE2	2.50	0.46
2:B:332:ALA:HB3	2:B:333:PRO:HD3	1.98	0.46
2:B:210:VAL:CG1	7:B:802:HEM:C2B	2.99	0.46
3:M:374:ALA:HB1	3:M:428:THR:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:332:ALA:HB3	2:D:333:PRO:HD3	1.96	0.46
3:N:517:LEU:HD12	3:N:517:LEU:O	2.16	0.46
2:D:39:LEU:HD23	2:D:46:PHE:CE2	2.50	0.46
3:N:98:SER:HB2	3:N:101:GLN:HG3	1.98	0.46
2:D:216:LEU:CD1	2:D:245:ILE:HG23	2.46	0.46
2:D:352:PHE:HB3	7:D:801:HEM:HBC1	1.97	0.45
2:D:398:VAL:O	2:D:402:LEU:HG	2.16	0.45
3:N:271:VAL:HG13	3:N:272:ASP:N	2.31	0.45
3:N:449:GLN:NE2	3:N:478:ALA:O	2.48	0.45
2:D:226:LEU:O	2:D:230:THR:OG1	2.20	0.45
2:D:231:GLY:O	2:D:299:ARG:HD3	2.16	0.45
3:M:84:THR:HB	3:M:85:PRO:HD2	1.98	0.45
1:A:91:PHE:O	1:A:94:PHE:HB3	2.16	0.45
2:D:83:GLU:OE1	2:D:234:ARG:NH1	2.49	0.45
3:M:246:TRP:HA	3:M:247:PRO:C	2.37	0.45
1:A:36:LEU:HD23	2:B:197:ARG:HG2	1.97	0.45
3:N:381:TYR:CD1	3:N:413:VAL:HG21	2.52	0.45
2:D:79:LEU:HB2	2:D:224:PHE:CE2	2.52	0.45
2:D:93:LEU:HD23	2:D:157:ASN:HB2	1.98	0.45
3:M:218:ILE:HG22	3:M:258:LEU:HD13	1.98	0.45
2:D:265:VAL:HB	2:D:266:PRO:HD2	1.97	0.45
3:N:218:ILE:HG22	3:N:258:LEU:HD13	1.98	0.45
2:D:17:LYS:N	2:D:18:PRO:HD2	2.32	0.45
3:M:147:LEU:HB2	3:M:148:PRO:CD	2.44	0.45
3:N:462:LYS:CG	3:N:463:TYR:N	2.80	0.44
3:N:62:PRO:O	3:N:67:ILE:HG21	2.15	0.44
2:D:341:THR:HG22	2:D:342:GLN:N	2.32	0.44
3:N:33:GLU:O	3:N:37:ASN:ND2	2.51	0.44
2:B:226:LEU:O	2:B:230:THR:OG1	2.23	0.44
3:M:471:TRP:CE3	3:M:517:LEU:HB2	2.52	0.44
1:A:137:THR:O	1:A:137:THR:HG23	2.18	0.44
1:C:137:THR:O	1:C:137:THR:HG23	2.17	0.44
2:D:382:SER:HB3	2:D:457:SER:O	2.18	0.44
3:N:370:PRO:HB3	3:N:387:THR:HB	1.98	0.44
2:B:216:LEU:CD1	2:B:245:ILE:HG23	2.48	0.44
2:B:382:SER:HB3	2:B:457:SER:O	2.18	0.44
2:D:338:THR:HB	2:D:343:LEU:HD23	1.99	0.43
3:M:271:VAL:HG13	3:M:272:ASP:N	2.33	0.43
3:M:370:PRO:HB3	3:M:387:THR:HB	2.00	0.43
2:D:131:THR:HB	2:D:144:LYS:HE2	1.99	0.43
2:D:144:LYS:HB3	2:D:189:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:THR:HB	2:B:343:LEU:HD23	1.99	0.43
1:C:115:PHE:HZ	4:C:201:HEC:HMC2	1.84	0.43
4:C:201:HEC:HBB3	4:C:201:HEC:HMB1	2.00	0.43
3:N:176:ASP:O	3:N:214:LYS:CE	2.64	0.43
3:N:239:TYR:CE1	3:N:312:ILE:HD12	2.54	0.43
2:B:10:PHE:CE2	2:B:82:GLU:HA	2.54	0.43
3:M:239:TYR:CE1	3:M:312:ILE:HD12	2.53	0.43
3:M:72:GLY:O	3:M:76:LEU:HG	2.18	0.43
3:N:72:GLY:O	3:N:76:LEU:HG	2.18	0.43
2:B:341:THR:HG22	2:B:342:GLN:N	2.34	0.43
2:B:37:MET:HB3	7:B:801:HEM:CMA	2.49	0.43
2:D:298:ARG:NH1	2:D:301:ASP:OD1	2.52	0.43
4:M:601:HEC:HMC1	4:M:601:HEC:CBC	2.49	0.43
3:M:75:TYR:CD1	3:M:75:TYR:C	2.91	0.43
1:A:137:THR:CG2	1:A:140:TRP:O	2.67	0.42
1:C:53:LYS:O	1:C:56:TRP:HB3	2.19	0.42
3:M:474:LEU:HD12	3:M:479:LYS:HD2	2.01	0.42
3:M:522:LYS:O	3:M:523:ASP:HB2	2.19	0.42
2:B:330:THR:HA	7:B:802:HEM:CMD	2.49	0.42
3:M:121:MET:HB2	3:N:274:GLN:HB3	2.00	0.42
3:M:403:LYS:HD2	3:M:403:LYS:H	1.84	0.42
1:C:137:THR:CG2	1:C:140:TRP:O	2.67	0.42
2:D:258:HIS:HE1	7:D:802:HEM:C4C	2.37	0.42
3:M:533:PHE:HZ	10:M:602:DHE:HAD1	1.83	0.42
3:M:291:HIS:HB3	3:M:292:PRO:HD2	2.01	0.42
4:N:601:HEC:HMB1	4:N:601:HEC:CBB	2.49	0.42
2:B:24:LEU:O	2:B:28:VAL:HG23	2.20	0.42
2:B:210:VAL:HG11	7:B:802:HEM:C2B	2.55	0.42
2:D:224:PHE:C	2:D:224:PHE:CD1	2.93	0.42
3:N:266:THR:HG21	3:N:282:VAL:HG22	2.01	0.42
1:A:53:LYS:O	1:A:56:TRP:HB3	2.20	0.42
3:M:266:THR:HG21	3:M:282:VAL:HG22	1.99	0.42
3:N:467:PRO:HG2	3:N:471:TRP:HE1	1.85	0.42
2:B:17:LYS:N	2:B:18:PRO:HD2	2.35	0.42
2:B:226:LEU:CD2	2:B:295:ILE:HG13	2.49	0.42
2:B:331:LEU:O	2:B:334:VAL:N	2.53	0.42
2:B:387:MET:O	2:B:391:TRP:HD1	2.02	0.42
3:M:425:PHE:CE1	10:M:602:DHE:CBD	3.03	0.42
3:N:65:PRO:O	3:N:69:GLN:HB2	2.19	0.42
2:D:392:LEU:HD13	2:D:449:ILE:HG22	2.02	0.41
3:N:138:PRO:HB3	3:N:142:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:77:GLU:OE2	3:N:103:THR:HG23	2.19	0.41
2:D:24:LEU:O	2:D:28:VAL:HG23	2.19	0.41
4:M:601:HEC:HMC1	4:M:601:HEC:HBC3	2.02	0.41
1:C:100:LYS:HD2	3:M:79:LEU:HD21	2.02	0.41
3:N:198:ARG:HH22	10:N:602:DHE:CBB	2.32	0.41
1:A:32:THR:OG1	2:B:268:TYR:OH	2.22	0.41
2:B:134:ARG:NH2	2:B:198:ASP:OD1	2.53	0.41
2:B:219:GLY:HA2	2:B:287:MET:HE3	2.03	0.41
3:N:533:PHE:HD1	3:N:538:THR:HG21	1.85	0.41
3:N:75:TYR:C	3:N:75:TYR:CD1	2.94	0.41
1:A:35:THR:O	1:A:39:ARG:HG3	2.20	0.41
2:B:349:HIS:CD2	7:B:801:HEM:NC	2.89	0.41
2:D:22:PHE:O	2:D:26:LEU:HG	2.21	0.41
2:D:283:PRO:O	2:D:287:MET:HG3	2.21	0.41
3:M:65:PRO:O	3:M:69:GLN:HB2	2.21	0.41
3:N:436:TYR:CE1	3:N:493:VAL:HG21	2.56	0.41
2:B:22:PHE:O	2:B:26:LEU:HG	2.20	0.41
3:M:436:TYR:CE1	3:M:493:VAL:HG21	2.55	0.41
3:M:62:PRO:O	3:M:67:ILE:HG21	2.20	0.41
3:N:113:PRO:HA	3:N:114:PRO:HD3	1.97	0.41
3:N:291:HIS:HB3	3:N:292:PRO:HD2	2.02	0.41
1:A:106:VAL:CG1	1:A:109:ARG:CD	2.99	0.41
1:A:140:TRP:CB	2:B:262:TRP:HB3	2.50	0.41
3:N:522:LYS:O	3:N:523:ASP:HB2	2.21	0.41
2:B:58:MET:HB3	12:B:911:HOH:O	2.20	0.41
3:N:147:LEU:HB2	3:N:148:PRO:CD	2.45	0.41
2:D:226:LEU:CD2	2:D:295:ILE:HG13	2.51	0.41
3:M:474:LEU:HD22	3:M:504:SER:O	2.20	0.41
1:C:74:PHE:HB2	2:D:53:PHE:CE1	2.56	0.41
1:C:91:PHE:O	1:C:94:PHE:HB3	2.20	0.41
2:D:90:SER:OG	2:D:92:LYS:HG2	2.20	0.40
1:C:11:ARG:HG3	2:D:242:TYR:CZ	2.56	0.40
3:M:532:LYS:HE2	3:M:532:LYS:HB2	1.95	0.40
2:B:283:PRO:O	2:B:287:MET:HG3	2.21	0.40
2:B:322:ALA:O	2:B:326:GLY:HA3	2.22	0.40
3:N:31:MET:HE2	3:N:36:PHE:HA	2.03	0.40
2:B:266:PRO:HB2	2:B:268:TYR:CE2	2.56	0.40
2:D:19:TYR:CZ	2:D:77:TYR:HE2	2.40	0.40
3:N:405:HIS:N	3:N:406:PRO:CD	2.85	0.40
1:C:49:VAL:HG13	1:C:128:PHE:HA	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:ARG:O	2:D:298:ARG:NH2[1_654]	2.12	0.08

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	140/146 (96%)	131 (94%)	9 (6%)	0	100	100
1	C	140/146 (96%)	131 (94%)	9 (6%)	0	100	100
2	B	447/465 (96%)	409 (92%)	36 (8%)	2 (0%)	34	69
2	D	447/465 (96%)	415 (93%)	30 (7%)	2 (0%)	34	69
3	M	536/568 (94%)	493 (92%)	40 (8%)	3 (1%)	25	64
3	N	536/568 (94%)	493 (92%)	41 (8%)	2 (0%)	34	69
All	All	2246/2358 (95%)	2072 (92%)	165 (7%)	9 (0%)	34	69

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	283	ALA
3	N	283	ALA
2	B	328	MET
2	D	328	MET
2	B	266	PRO
2	D	266	PRO
3	N	483	GLN
3	M	132	VAL
3	M	483	GLN

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	116/120 (97%)	115 (99%)	1 (1%)	78	91
1	C	116/120 (97%)	114 (98%)	2 (2%)	60	83
2	B	360/371 (97%)	349 (97%)	11 (3%)	40	72
2	D	360/371 (97%)	351 (98%)	9 (2%)	47	77
3	M	453/476 (95%)	445 (98%)	8 (2%)	59	82
3	N	453/476 (95%)	444 (98%)	9 (2%)	55	80
All	All	1858/1934 (96%)	1818 (98%)	40 (2%)	52	79

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	PHE
2	B	240	TRP
2	B	258	HIS
2	B	297	ARG
2	B	298	ARG
2	B	352	PHE
2	B	372	ARG
2	B	382	SER
2	B	383	GLN
2	B	401	THR
2	B	416	ARG
2	B	440	ARG
1	C	15	PHE
1	C	39	ARG
2	D	144	LYS
2	D	258	HIS
2	D	298	ARG
2	D	301	ASP
2	D	305	ARG
2	D	352	PHE
2	D	382	SER
2	D	383	GLN

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Mol	Chain	Res	Type
2	D	416	ARG
3	M	31	MET
3	M	169	LYS
3	M	198	ARG
3	M	229	SER
3	M	333	SER
3	M	427	LYS
3	M	437	VAL
3	M	525	ARG
3	N	31	MET
3	N	45	GLN
3	N	90	ASN
3	N	137	ARG
3	N	168	SER
3	N	198	ARG
3	N	213	THR
3	N	229	SER
3	N	437	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	HEM	D	801	2,5	27,50,50	2.27	6 (22%)	17,82,82	2.32	6 (35%)
10	DHE	N	602	3	38,56,56	5.27	22 (57%)	37,94,94	5.29	19 (51%)
6	10M	D	805	-	34,34,34	0.83	0	44,45,45	1.28	5 (11%)
4	HEC	N	601	3	26,50,50	2.14	7 (26%)	18,82,82	2.35	6 (33%)
4	HEC	M	601	3	26,50,50	2.25	6 (23%)	18,82,82	2.09	5 (27%)
7	HEM	B	801	2,5	27,50,50	2.23	5 (18%)	17,82,82	2.50	6 (35%)
7	HEM	B	802	9,2,5	27,50,50	2.08	6 (22%)	17,82,82	2.35	5 (29%)
4	HEC	A	201	1	26,50,50	2.23	4 (15%)	18,82,82	2.01	5 (27%)
10	DHE	M	602	3	38,56,56	5.24	23 (60%)	37,94,94	5.33	20 (54%)
7	HEM	D	802	9,2,5	27,50,50	2.11	5 (18%)	17,82,82	2.42	6 (35%)
6	10M	C	203	-	34,34,34	0.59	0	44,45,45	0.83	1 (2%)
6	10M	A	203	-	34,34,34	0.54	0	44,45,45	0.82	0
4	HEC	C	201	1	26,50,50	2.09	3 (11%)	18,82,82	2.05	6 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HEM	D	801	2,5	-	0/6/54/54	-
10	DHE	N	602	3	-	4/12/108/108	-
6	10M	D	805	-	-	10/19/59/59	0/2/2/2
4	HEC	N	601	3	-	0/6/54/54	-
4	HEC	M	601	3	-	0/6/54/54	-
7	HEM	B	801	2,5	-	0/6/54/54	-
7	HEM	B	802	9,2,5	-	2/6/54/54	-
4	HEC	A	201	1	-	0/6/54/54	-
10	DHE	M	602	3	-	4/12/108/108	-
7	HEM	D	802	9,2,5	-	0/6/54/54	-
6	10M	C	203	-	-	4/19/59/59	0/2/2/2
6	10M	A	203	-	-	4/19/59/59	0/2/2/2
4	HEC	C	201	1	-	1/6/54/54	-

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	602	DHE	C4B-NB	-14.13	1.35	1.49
10	N	602	DHE	C4C-NC	-13.34	1.36	1.49
10	M	602	DHE	C4C-NC	-12.92	1.36	1.49
10	N	602	DHE	C4B-NB	-12.84	1.36	1.49
10	M	602	DHE	C1C-NC	-10.80	1.34	1.49
10	N	602	DHE	C1B-NB	-10.79	1.35	1.49
10	N	602	DHE	C1C-NC	-10.12	1.35	1.49
10	M	602	DHE	C1A-C2A	8.91	1.50	1.38
10	M	602	DHE	C1B-NB	-8.86	1.37	1.49
10	N	602	DHE	C1A-C2A	8.38	1.49	1.38
10	N	602	DHE	C1D-C2D	7.97	1.49	1.38
10	N	602	DHE	C4A-C3A	7.75	1.48	1.38
10	M	602	DHE	C4D-C3D	7.67	1.48	1.38
10	N	602	DHE	C4D-C3D	7.49	1.48	1.38
10	M	602	DHE	C1D-C2D	7.13	1.47	1.38
10	M	602	DHE	C4A-C3A	6.58	1.47	1.38
4	A	201	HEC	C3B-C2B	-6.34	1.34	1.40
4	C	201	HEC	C3C-C2C	-6.18	1.34	1.40
10	M	602	DHE	C3B-C2B	-6.04	1.45	1.52
7	D	801	HEM	C3B-C2B	-5.96	1.32	1.40
4	M	601	HEC	C3B-C2B	-5.89	1.34	1.40
4	N	601	HEC	C3C-C2C	-5.81	1.34	1.40
7	B	801	HEM	C3C-C2C	-5.64	1.32	1.40
4	C	201	HEC	C3B-C2B	-5.64	1.34	1.40
10	M	602	DHE	CHA-C4D	-5.51	1.45	1.51
10	N	602	DHE	CHA-C1A	-5.51	1.45	1.51
4	M	601	HEC	C3C-C2C	-5.49	1.35	1.40
7	B	801	HEM	C3B-C2B	-5.34	1.33	1.40
7	D	801	HEM	C3C-C2C	-5.34	1.33	1.40
4	A	201	HEC	C3C-C2C	-5.27	1.35	1.40
10	N	602	DHE	C3B-C2B	-5.26	1.46	1.52
10	M	602	DHE	CHA-C1A	-5.19	1.45	1.51
7	D	801	HEM	C3D-C2D	5.18	1.53	1.37
4	N	601	HEC	C3D-C2D	5.17	1.53	1.37
10	N	602	DHE	OMC-C2C	5.15	1.30	1.21
7	D	802	HEM	C3D-C2D	5.14	1.52	1.37
7	B	801	HEM	C3D-C2D	5.12	1.52	1.37
7	B	802	HEM	C3D-C2D	5.09	1.52	1.37
10	M	602	DHE	OMC-C2C	5.07	1.30	1.21
7	D	802	HEM	C3C-C2C	-5.05	1.33	1.40
4	M	601	HEC	C3D-C2D	4.90	1.52	1.37
10	M	602	DHE	OMB-C2B	4.86	1.29	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	HEC	C3D-C2D	4.82	1.51	1.37
7	B	802	HEM	C3C-C2C	-4.79	1.33	1.40
7	B	802	HEM	C3B-C2B	-4.77	1.33	1.40
10	N	602	DHE	CHA-C4D	-4.75	1.46	1.51
7	D	802	HEM	C3B-C2B	-4.73	1.33	1.40
10	N	602	DHE	CHB-C1B	-4.43	1.45	1.53
10	N	602	DHE	OMB-C2B	4.10	1.28	1.21
10	N	602	DHE	C3C-C2C	-4.00	1.47	1.52
10	N	602	DHE	C2A-C3A	3.91	1.49	1.37
4	N	601	HEC	C3B-C2B	-3.90	1.36	1.40
4	C	201	HEC	C3D-C2D	3.84	1.49	1.37
10	N	602	DHE	C1B-C2B	-3.82	1.44	1.50
10	M	602	DHE	C3C-C2C	-3.68	1.48	1.52
10	M	602	DHE	C3C-C4C	-3.47	1.50	1.55
10	M	602	DHE	C2A-C3A	3.39	1.47	1.37
10	M	602	DHE	CHB-C1B	-3.31	1.47	1.53
10	N	602	DHE	C3C-C4C	-3.28	1.50	1.55
7	D	802	HEM	C3B-CAB	3.18	1.54	1.47
7	B	801	HEM	C3C-CAC	3.13	1.54	1.47
7	B	802	HEM	C3C-CAC	3.06	1.54	1.47
10	N	602	DHE	C3D-C2D	2.94	1.46	1.37
7	B	802	HEM	C3B-CAB	2.90	1.53	1.47
7	B	801	HEM	C3B-CAB	2.89	1.53	1.47
10	M	602	DHE	CHD-C4C	-2.86	1.46	1.54
7	D	801	HEM	CAA-C2A	2.86	1.56	1.52
10	M	602	DHE	C1B-C2B	-2.85	1.45	1.50
7	D	802	HEM	C3C-CAC	2.79	1.53	1.47
10	M	602	DHE	C3B-C4B	-2.69	1.51	1.55
4	A	201	HEC	C3B-C4B	2.63	1.47	1.43
7	D	801	HEM	C3B-CAB	2.59	1.53	1.47
10	M	602	DHE	C3D-C2D	2.35	1.44	1.37
10	N	602	DHE	C3B-C4B	-2.33	1.52	1.55
10	N	602	DHE	CHC-C4B	-2.31	1.46	1.52
7	D	801	HEM	C3C-CAC	2.31	1.52	1.47
10	M	602	DHE	CAB-C3B	-2.31	1.52	1.56
10	N	602	DHE	CHD-C4C	-2.24	1.48	1.54
4	M	601	HEC	C1D-ND	2.21	1.40	1.36
10	M	602	DHE	CHB-C4A	-2.19	1.45	1.51
4	N	601	HEC	CAD-C3D	2.17	1.55	1.52
7	B	802	HEM	CAA-C2A	2.15	1.55	1.52
4	M	601	HEC	C3B-C4B	2.13	1.46	1.43
4	N	601	HEC	C3C-C4C	2.08	1.46	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	601	HEC	C4D-ND	2.05	1.40	1.36
4	N	601	HEC	CMA-C3A	2.04	1.56	1.51
4	N	601	HEC	CMB-C2B	2.03	1.56	1.51

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	602	DHE	C3C-C4C-NC	17.74	120.27	104.67
10	N	602	DHE	C3B-C4B-NB	15.75	118.52	104.67
10	N	602	DHE	C3C-C4C-NC	15.73	118.50	104.67
10	M	602	DHE	C3B-C4B-NB	12.32	115.50	104.67
10	N	602	DHE	CHC-C1C-NC	11.88	125.72	110.94
10	M	602	DHE	CHC-C1C-NC	10.89	124.47	110.94
10	M	602	DHE	CHB-C1B-NB	9.09	127.89	110.75
10	M	602	DHE	C4C-C3C-C2C	-8.41	92.58	100.71
10	N	602	DHE	CHB-C1B-NB	8.02	125.89	110.75
7	B	802	HEM	CAD-CBD-CGD	-7.88	99.45	112.67
10	N	602	DHE	CHA-C4D-C3D	-7.72	120.36	129.68
10	N	602	DHE	C4B-C3B-C2B	-7.50	93.45	100.71
10	M	602	DHE	CHA-C4D-C3D	-7.20	120.99	129.68
7	B	801	HEM	CBD-CAD-C3D	-6.78	99.98	112.48
10	N	602	DHE	C4C-C3C-C2C	-6.29	94.62	100.71
10	M	602	DHE	CHD-C1D-C2D	-5.69	119.60	129.45
10	M	602	DHE	CAD-C3D-C4D	5.63	131.25	127.30
10	M	602	DHE	CHA-C1A-C2A	-5.62	122.90	129.68
4	C	201	HEC	CBD-CAD-C3D	-5.42	102.49	112.49
7	D	802	HEM	CBA-CAA-C2A	-5.06	103.15	112.49
7	D	801	HEM	CBD-CAD-C3D	-5.00	103.26	112.48
4	N	601	HEC	CMB-C2B-C1B	-4.87	120.98	128.46
7	D	801	HEM	C4C-C3C-C2C	4.78	110.24	106.90
10	N	602	DHE	CBA-CAA-C2A	4.68	121.12	112.49
4	N	601	HEC	CMB-C2B-C3B	4.55	131.17	125.82
4	A	201	HEC	CBA-CAA-C2A	-4.51	104.18	112.48
4	M	601	HEC	CBD-CAD-C3D	-4.49	104.20	112.49
10	M	602	DHE	CHC-C1C-C2C	4.47	128.66	114.70
10	N	602	DHE	CHD-C1D-C2D	-4.45	121.74	129.45
4	M	601	HEC	CMC-C2C-C1C	-4.35	121.78	128.46
4	N	601	HEC	CBD-CAD-C3D	-4.34	104.48	112.49
7	D	802	HEM	CAD-CBD-CGD	-4.31	105.43	112.67
10	M	602	DHE	C4D-CHA-C1A	4.29	123.34	112.87
10	N	602	DHE	CHA-C1A-C2A	-4.29	124.50	129.68
4	A	201	HEC	C1D-C2D-C3D	-4.23	104.05	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	802	HEM	CMB-C2B-C3B	4.16	132.46	124.68
7	B	801	HEM	C4C-C3C-C2C	4.15	109.80	106.90
10	M	602	DHE	C4B-C3B-C2B	-3.92	96.92	100.71
4	N	601	HEC	CMC-C2C-C1C	-3.88	122.49	128.46
10	N	602	DHE	CHB-C4A-C3A	-3.88	122.74	129.45
4	M	601	HEC	CMB-C2B-C1B	-3.84	122.57	128.46
6	D	805	10M	C18-C19-C20	3.80	117.45	110.82
10	N	602	DHE	CHC-C1C-C2C	3.69	126.23	114.70
10	N	602	DHE	CAD-C3D-C4D	3.69	129.89	127.30
10	M	602	DHE	CHB-C4A-C3A	-3.62	123.19	129.45
10	M	602	DHE	C1D-C2D-C3D	-3.61	101.97	105.81
4	A	201	HEC	CBD-CAD-C3D	-3.60	105.86	112.49
10	M	602	DHE	CGC-C3C-C2C	3.57	115.39	106.42
10	M	602	DHE	CAA-CBA-CGA	-3.55	106.71	112.67
7	D	802	HEM	CMD-C2D-C1D	3.53	133.89	128.46
10	N	602	DHE	CHB-C1B-C2B	3.49	124.77	114.47
10	N	602	DHE	C4D-CHA-C1A	3.47	121.34	112.87
10	M	602	DHE	OMC-C2C-C3C	-3.44	120.84	125.59
10	M	602	DHE	CHB-C1B-C2B	3.41	124.53	114.47
4	C	201	HEC	CMB-C2B-C1B	-3.37	123.29	128.46
6	D	805	10M	C19-C18-C16	3.27	116.08	110.24
7	D	801	HEM	C4A-C3A-C2A	3.21	109.23	107.00
4	A	201	HEC	CMB-C2B-C1B	-3.18	123.57	128.46
7	D	802	HEM	CMD-C2D-C3D	-3.14	119.03	124.94
4	M	601	HEC	CMC-C2C-C3C	3.12	129.49	125.82
7	B	801	HEM	CMD-C2D-C1D	3.03	133.12	128.46
7	D	801	HEM	CMD-C2D-C1D	2.96	133.02	128.46
6	D	805	10M	C22-C21-C14	2.94	116.39	109.68
10	M	602	DHE	C1C-CHC-C4B	2.93	124.76	116.16
4	C	201	HEC	C1D-C2D-C3D	-2.85	105.01	107.00
10	N	602	DHE	C4A-C3A-C2A	2.79	108.78	105.81
4	M	601	HEC	CMB-C2B-C3B	2.79	129.10	125.82
7	B	802	HEM	CMA-C3A-C4A	-2.77	124.20	128.46
7	B	801	HEM	CAD-CBD-CGD	2.77	117.32	112.67
4	N	601	HEC	CAA-CBA-CGA	-2.71	108.13	112.67
7	B	801	HEM	CMA-C3A-C4A	-2.67	124.36	128.46
7	D	801	HEM	CAD-CBD-CGD	2.62	117.07	112.67
6	D	805	10M	C15-O3-C14	-2.59	111.56	117.96
7	B	802	HEM	CMB-C2B-C3B	2.56	129.47	124.68
10	N	602	DHE	C4D-C3D-C2D	-2.50	102.20	105.93
7	B	802	HEM	CMC-C2C-C3C	2.47	129.30	124.68
4	C	201	HEC	CAD-CBD-CGD	-2.39	108.67	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	801	HEM	CMD-C2D-C3D	-2.39	120.44	124.94
7	D	802	HEM	CMC-C2C-C3C	2.39	129.14	124.68
7	B	802	HEM	C4A-C3A-C2A	2.32	108.61	107.00
6	D	805	10M	C15-C20-C19	2.32	114.82	110.00
4	C	201	HEC	CMB-C2B-C3B	2.29	128.51	125.82
4	N	601	HEC	CMC-C2C-C3C	2.29	128.51	125.82
7	D	801	HEM	C3C-C4C-NC	-2.26	106.69	110.94
4	C	201	HEC	CAA-CBA-CGA	-2.22	108.95	112.67
10	N	602	DHE	CGC-C3C-C2C	2.21	111.98	106.42
10	M	602	DHE	OMB-C2B-C3B	-2.16	122.60	125.59
10	N	602	DHE	CGB-C3B-CAB	-2.15	107.24	110.77
4	A	201	HEC	CMC-C2C-C1C	-2.09	125.25	128.46
6	C	203	10M	O10-C22-C11	2.01	113.96	110.27

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	N	602	DHE	C2B-C3B-CAB-CBB
10	N	602	DHE	CGB-C3B-CAB-CBB
10	N	602	DHE	C4B-C3B-CAB-CBB
10	N	602	DHE	C2C-C3C-CAC-CBC
10	M	602	DHE	C2B-C3B-CAB-CBB
10	M	602	DHE	CGB-C3B-CAB-CBB
10	M	602	DHE	C4B-C3B-CAB-CBB
6	D	805	10M	C18-C16-C17-O5
6	C	203	10M	C7-C8-C9-C10
6	A	203	10M	C7-C8-C9-C10
6	D	805	10M	O4-C16-C17-O5
6	D	805	10M	C2-C3-C4-C5
6	D	805	10M	C3-C4-C5-C6
6	D	805	10M	C4-C5-C6-C7
6	D	805	10M	C6-C7-C8-C9
6	D	805	10M	C5-C6-C7-C8
6	A	203	10M	C6-C7-C8-C9
6	C	203	10M	C9-C10-S-C11
6	A	203	10M	C9-C10-S-C11
6	D	805	10M	C1-C2-C3-C4
7	B	802	HEM	C1A-C2A-CAA-CBA
7	B	802	HEM	C3A-C2A-CAA-CBA
6	D	805	10M	C21-C14-O3-C15
4	C	201	HEC	C2A-CAA-CBA-CGA

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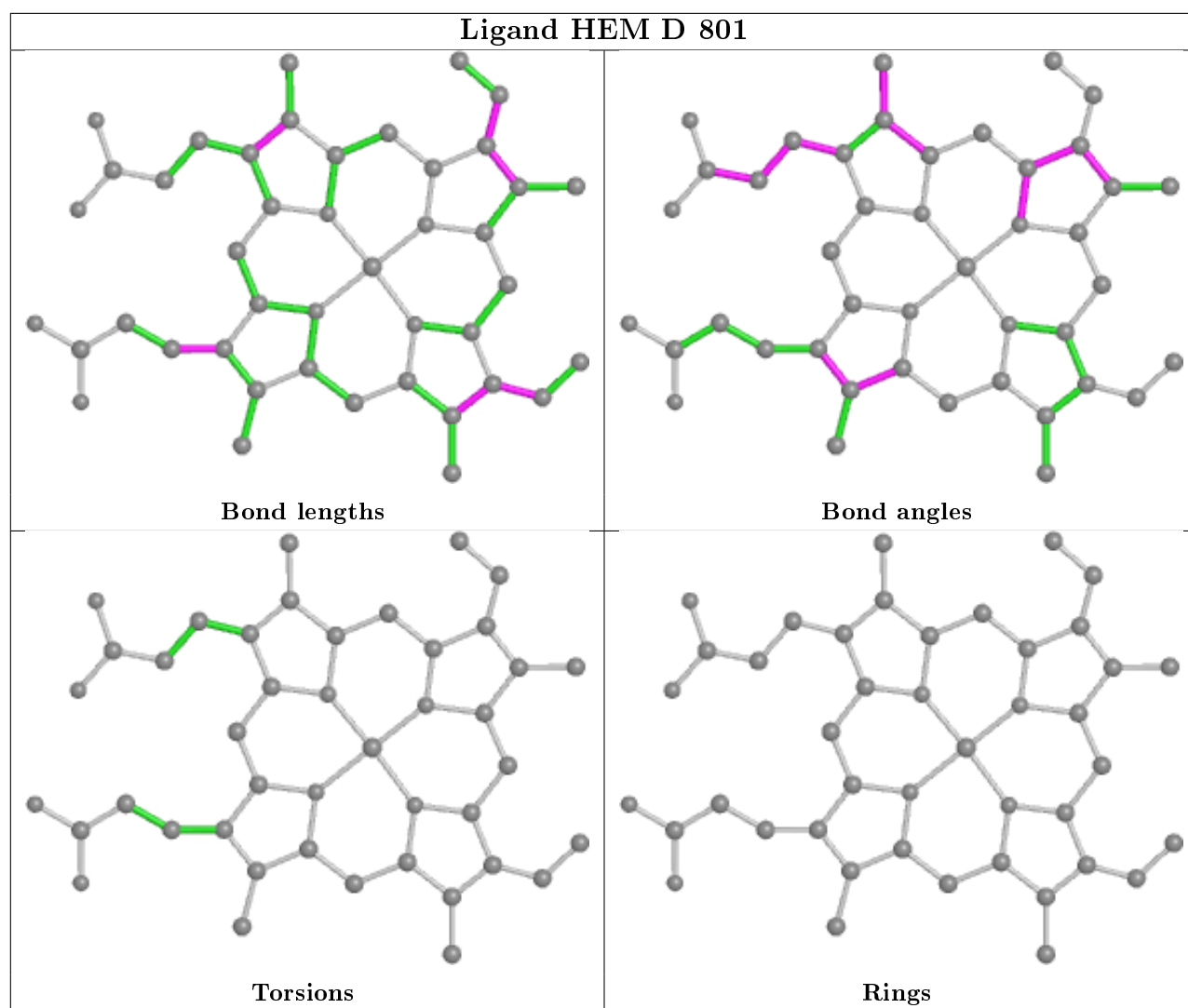
Mol	Chain	Res	Type	Atoms
6	A	203	10M	C14-C12-C13-O2
6	D	805	10M	C12-C14-O3-C15
10	M	602	DHE	CGC-C3C-CAC-CBC
6	C	203	10M	C6-C7-C8-C9
6	C	203	10M	C22-C11-S-C10

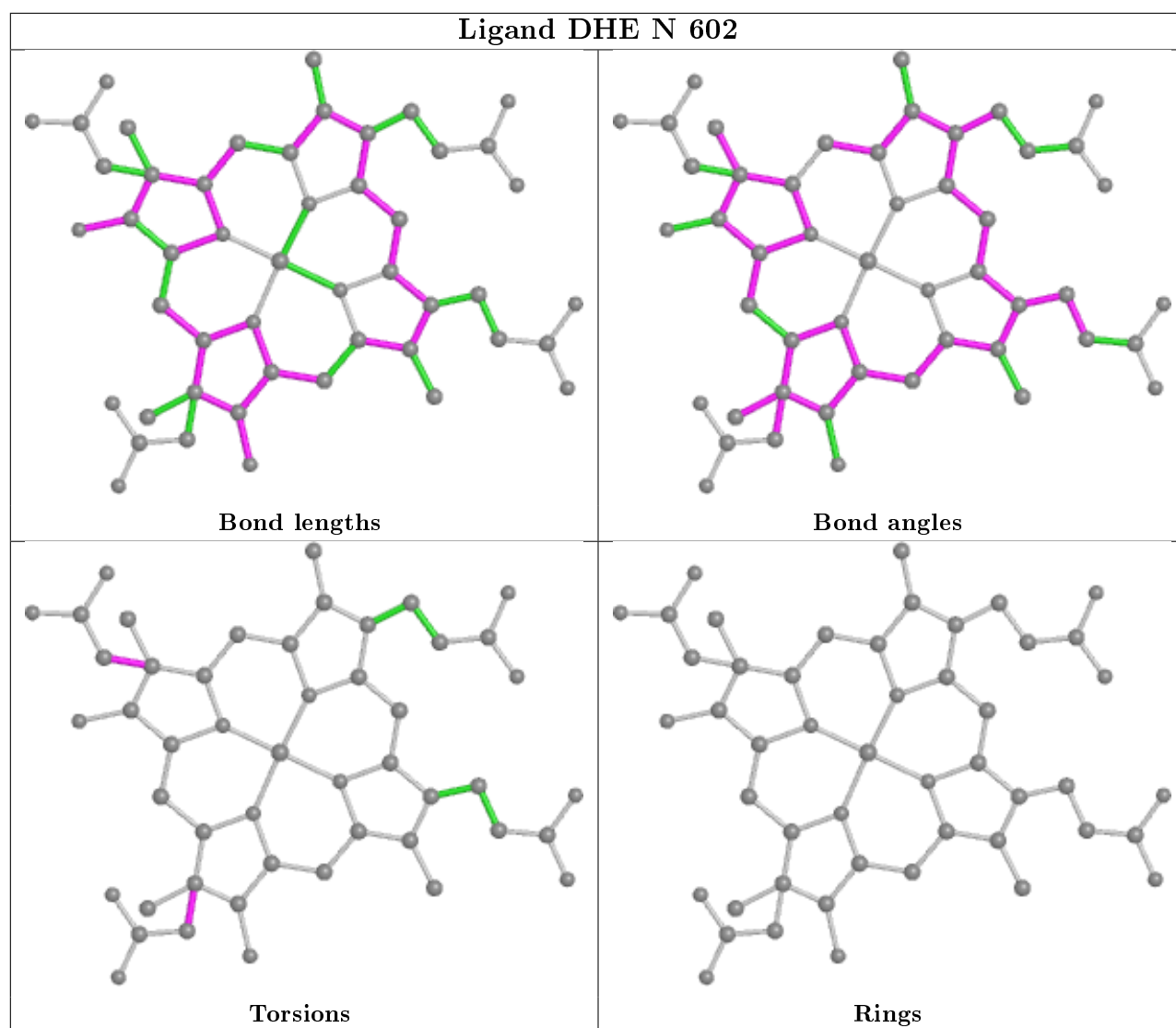
There are no ring outliers.

10 monomers are involved in 43 short contacts:

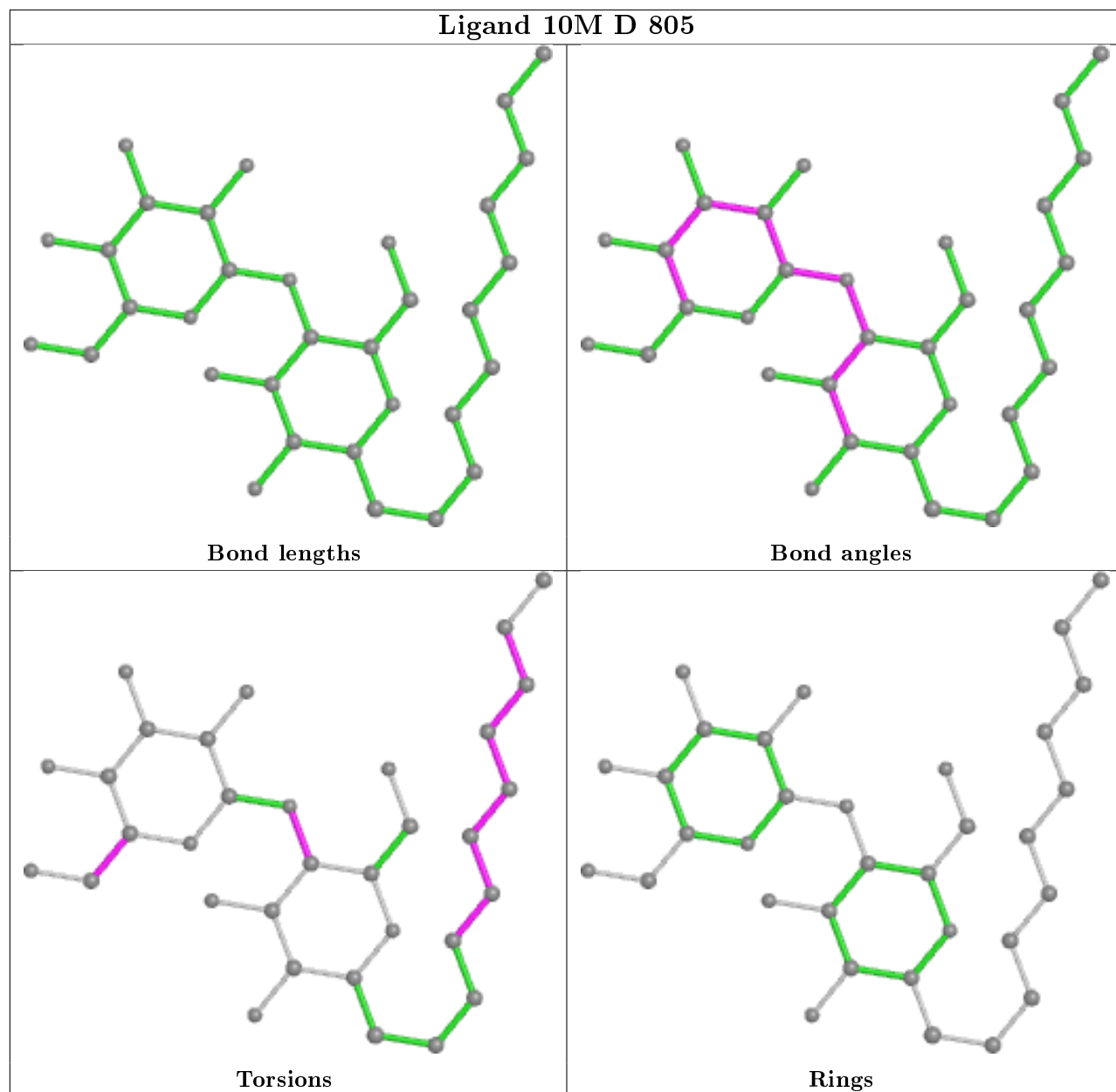
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	801	HEM	4	0
10	N	602	DHE	3	0
4	N	601	HEC	4	0
4	M	601	HEC	4	0
7	B	801	HEM	5	0
7	B	802	HEM	3	0
4	A	201	HEC	6	0
10	M	602	DHE	7	0
7	D	802	HEM	2	0
4	C	201	HEC	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

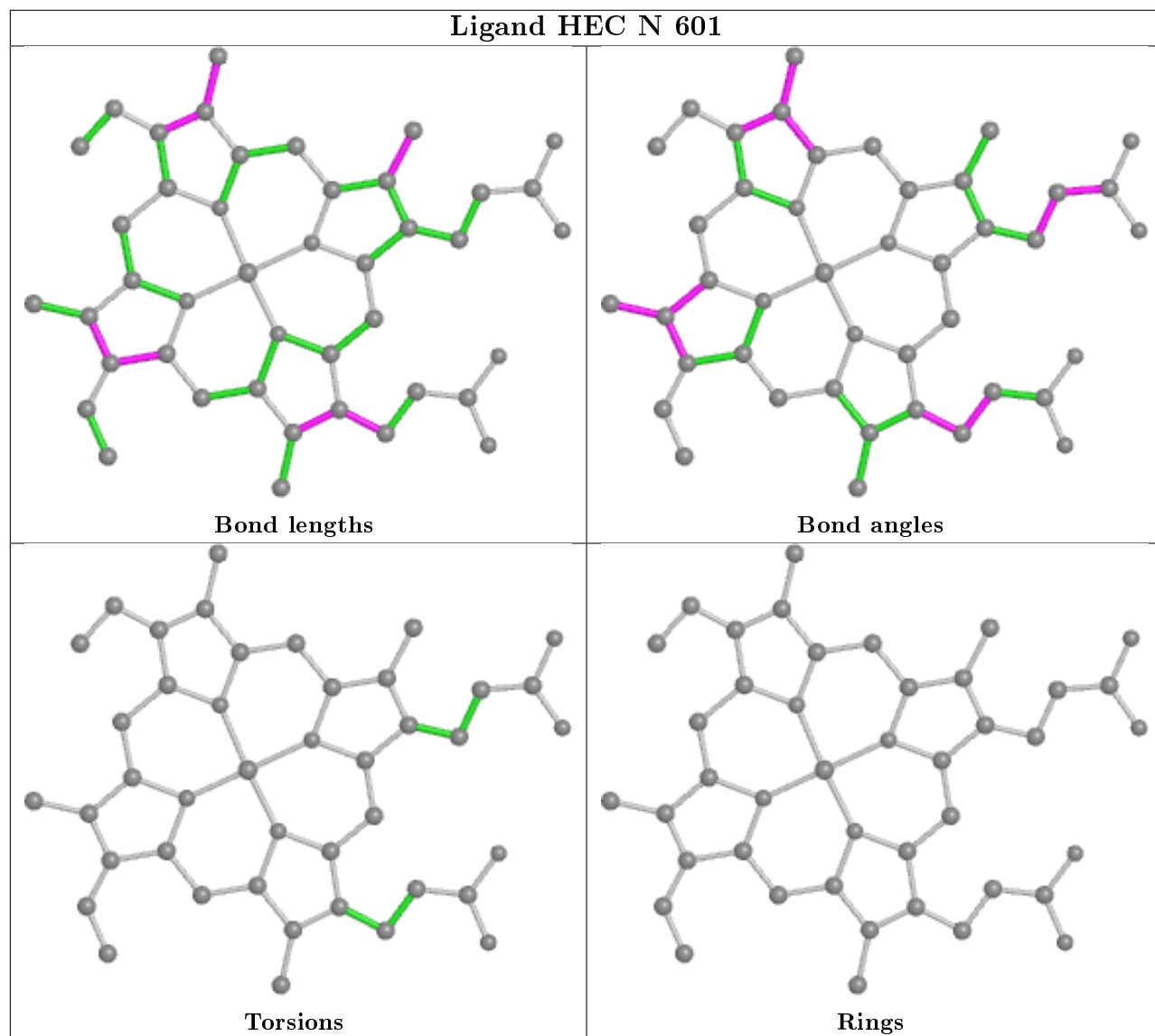


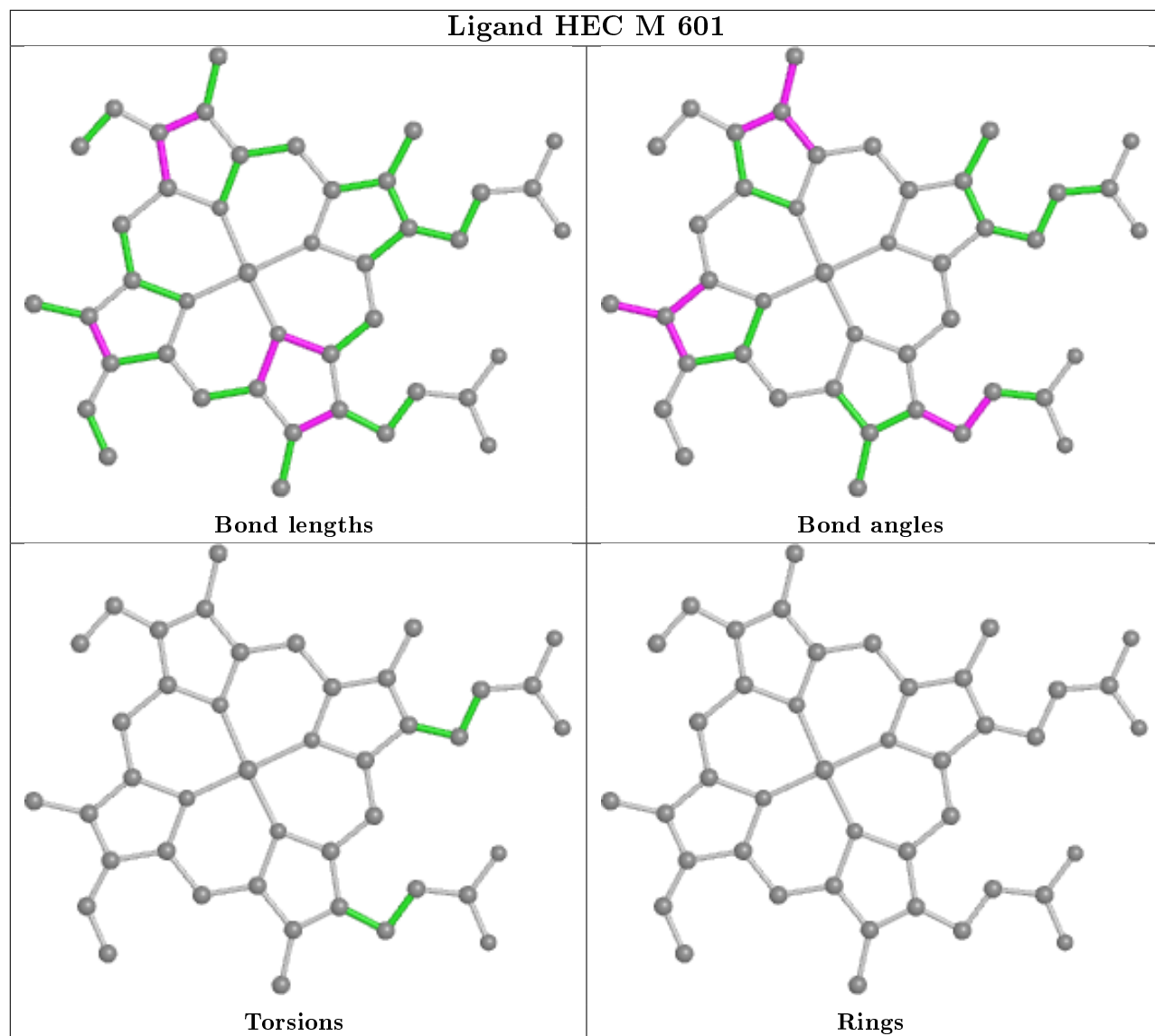


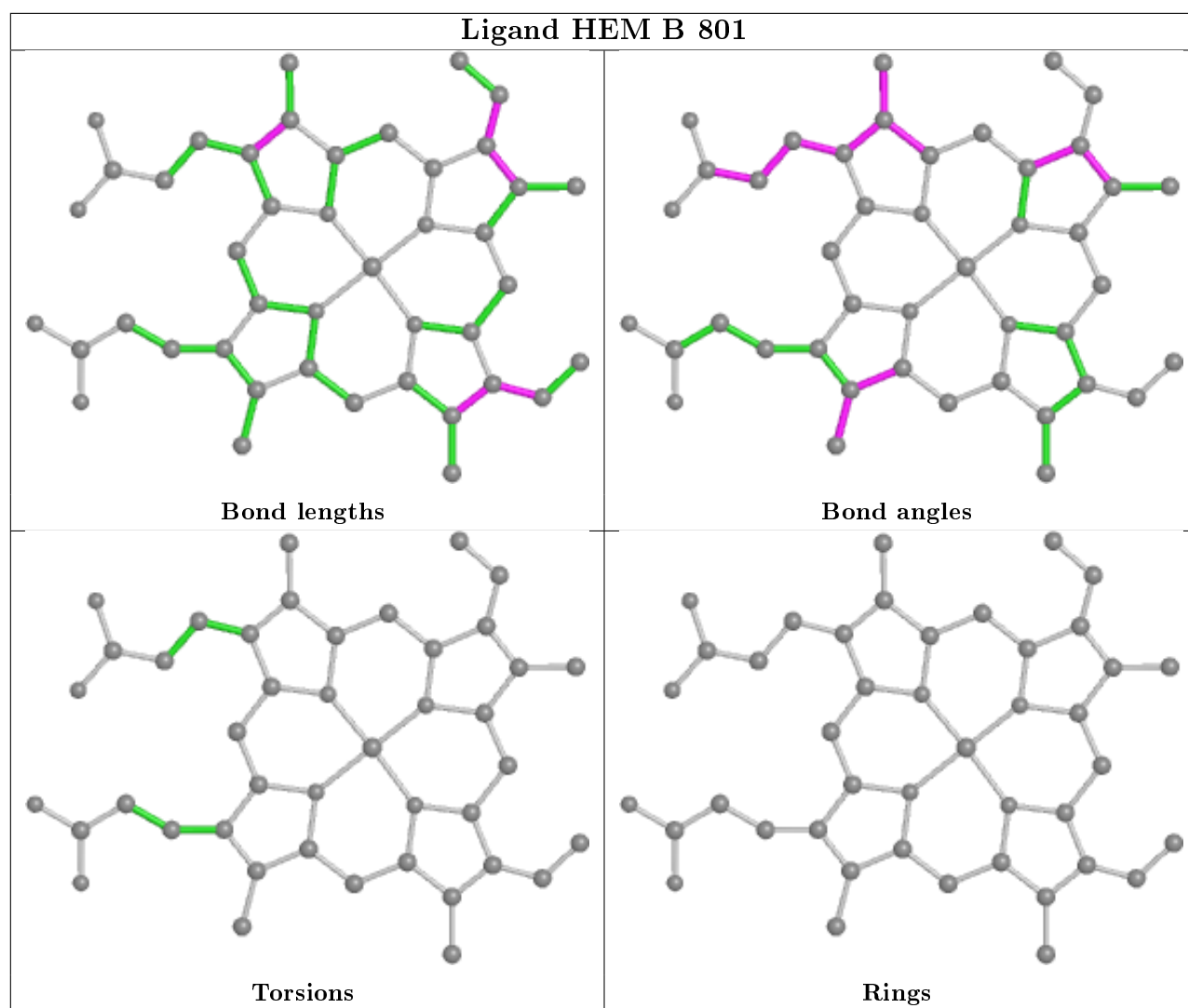
## Ligand 10M D 805

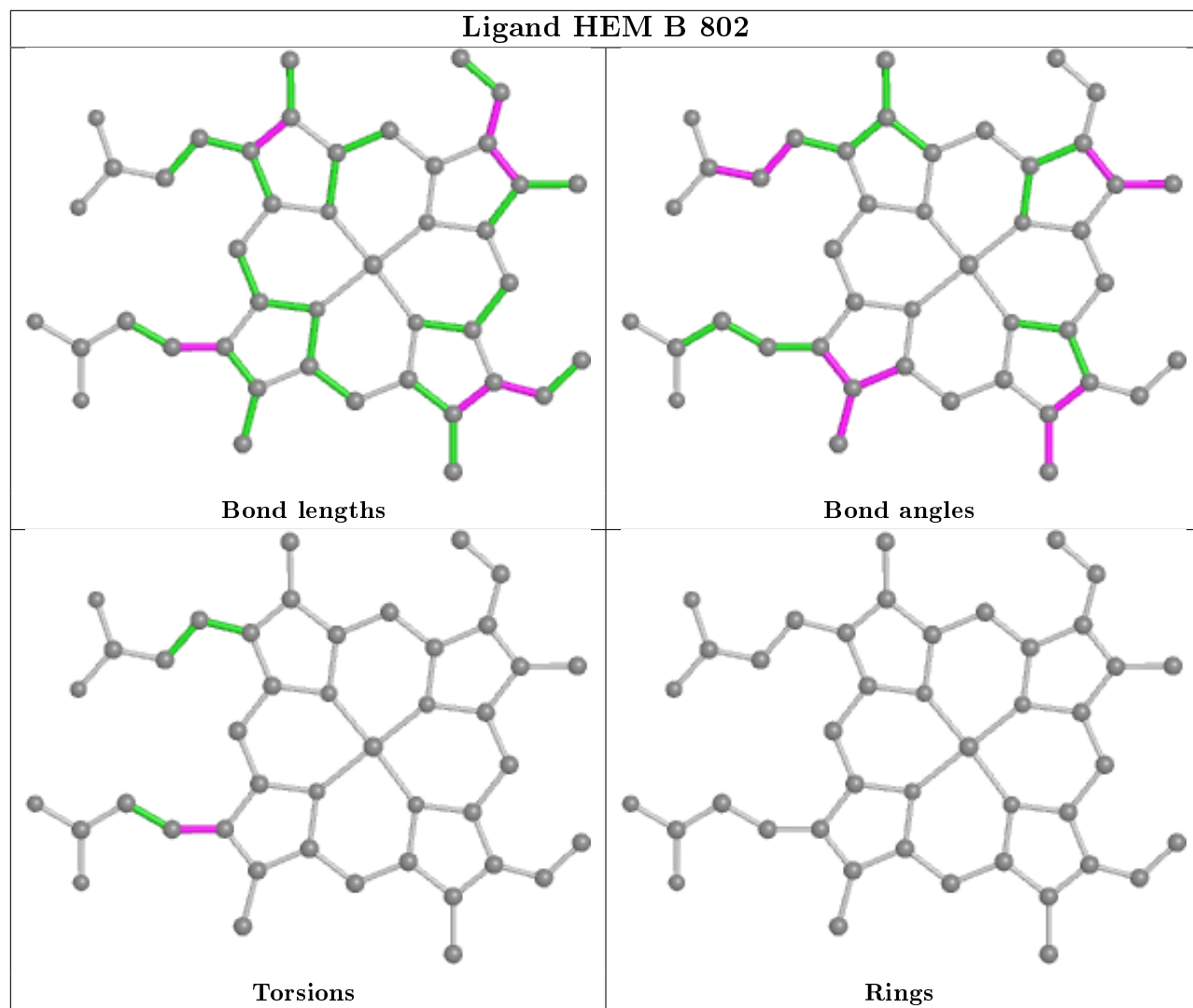




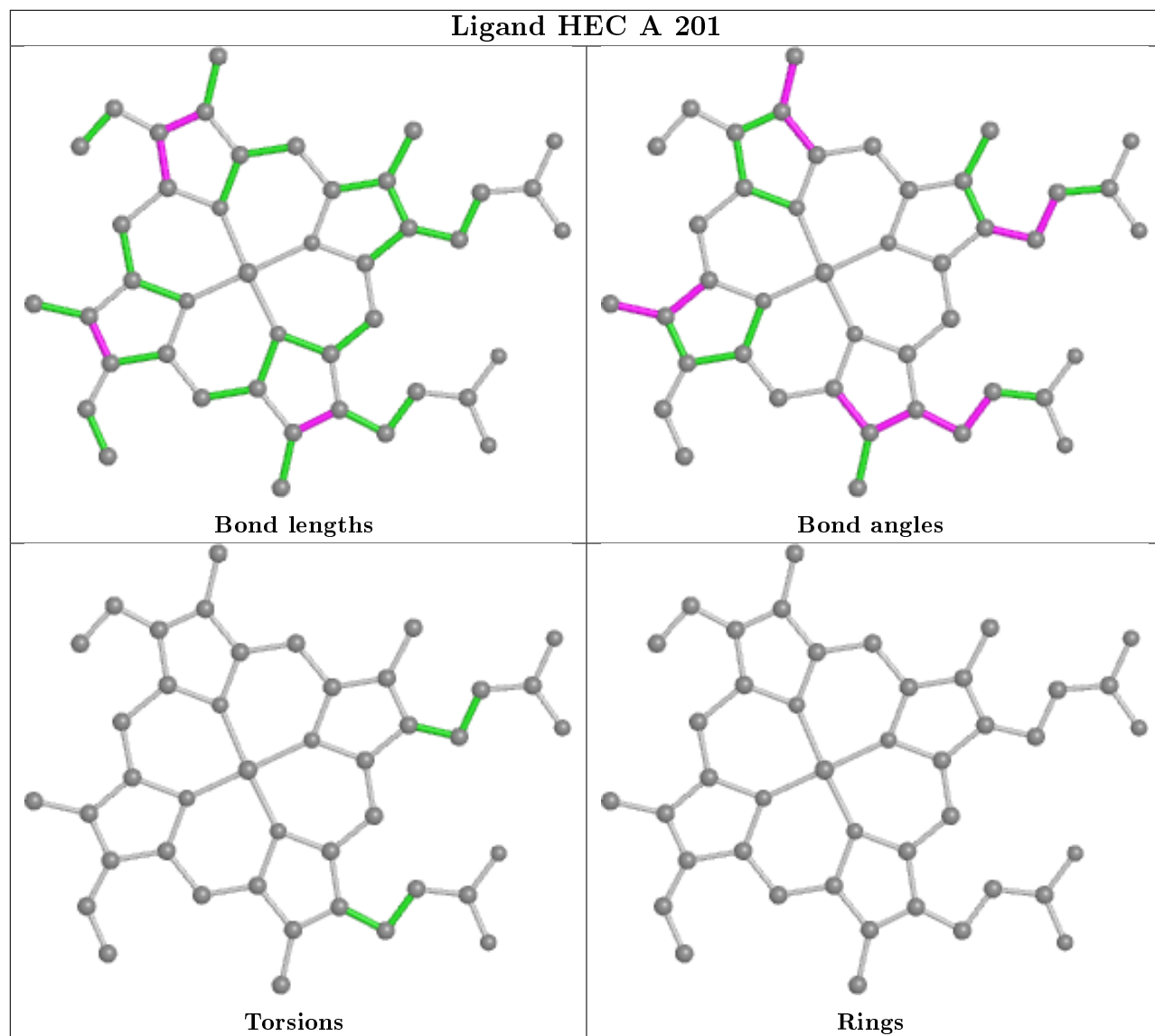


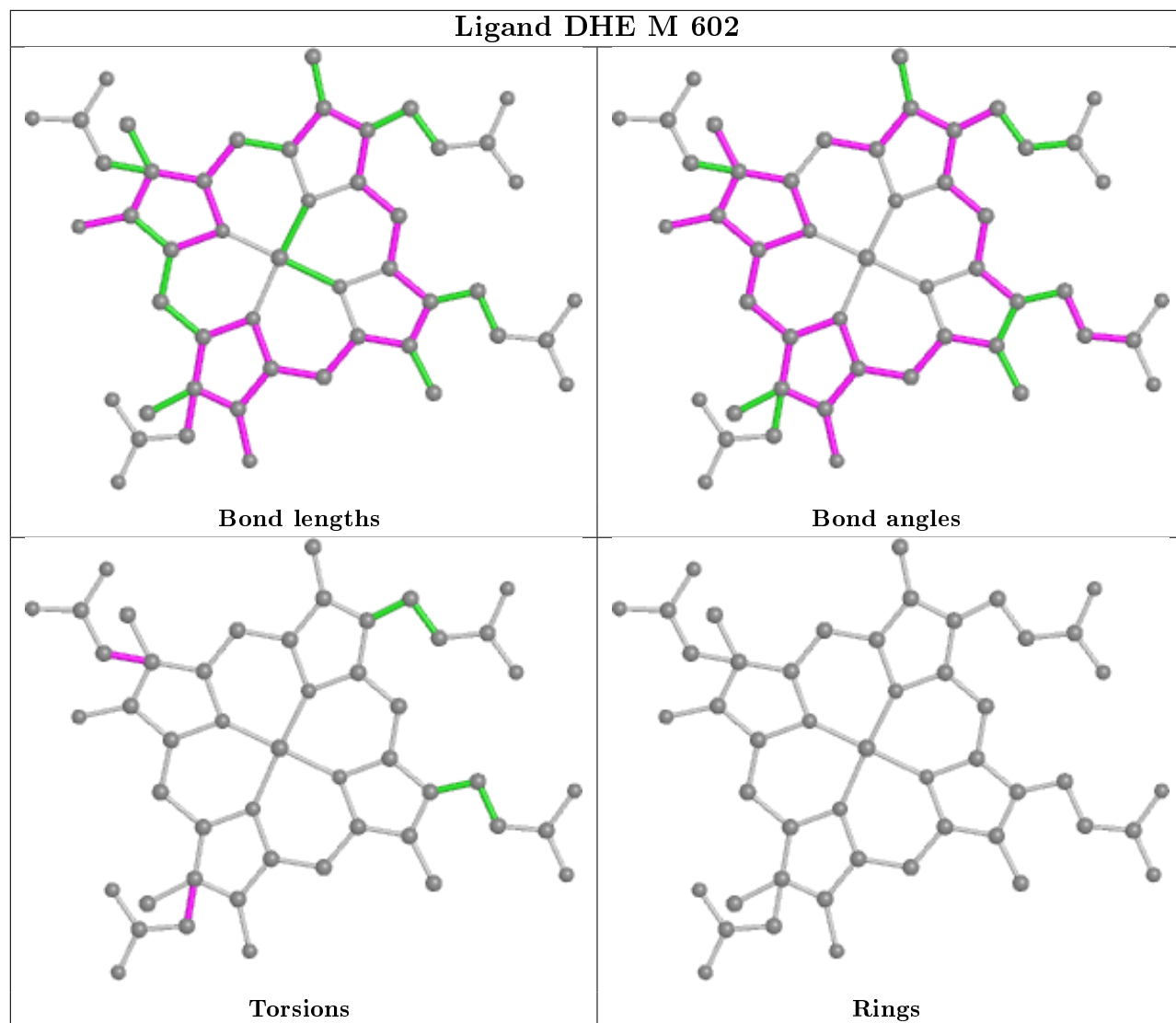


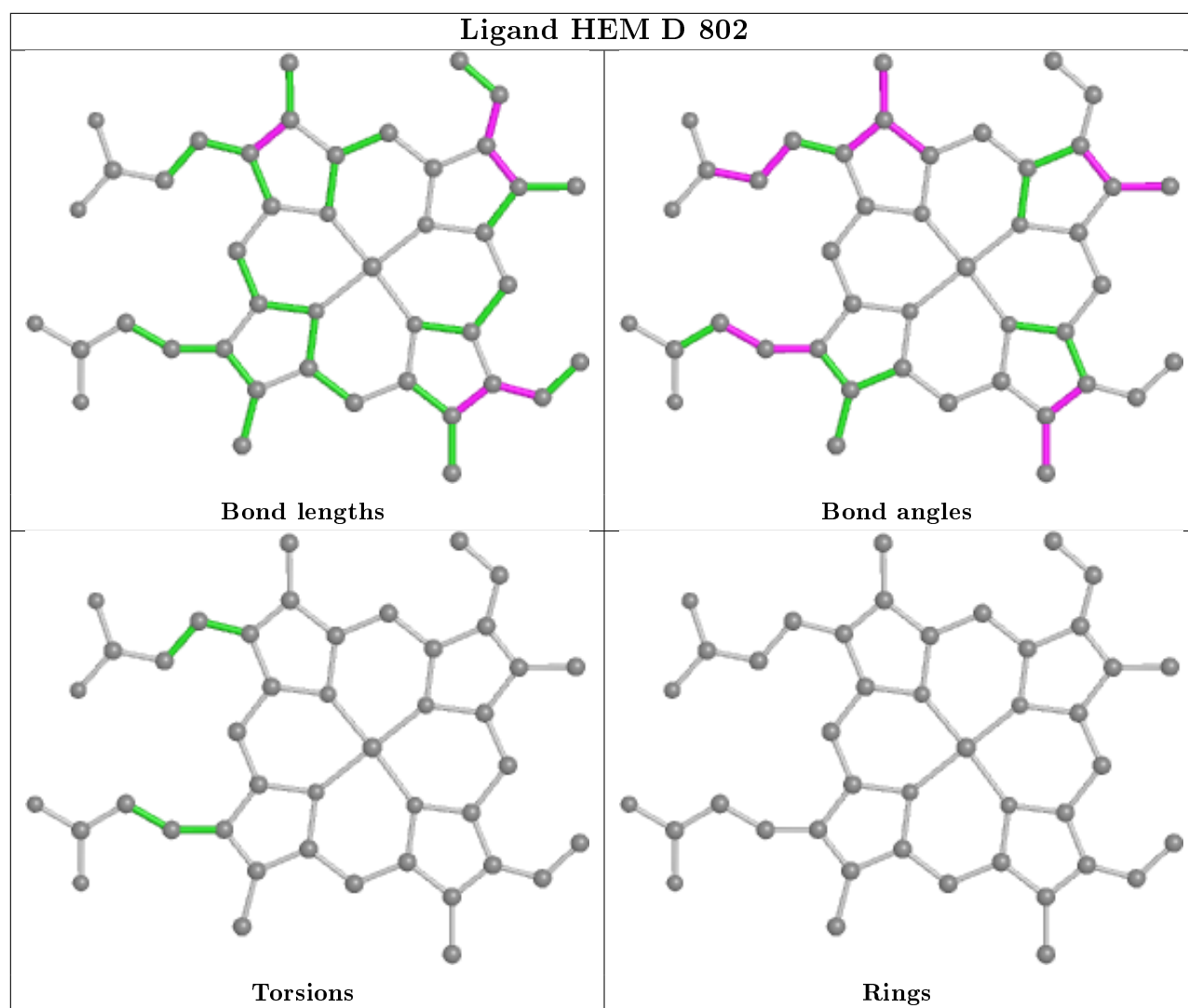




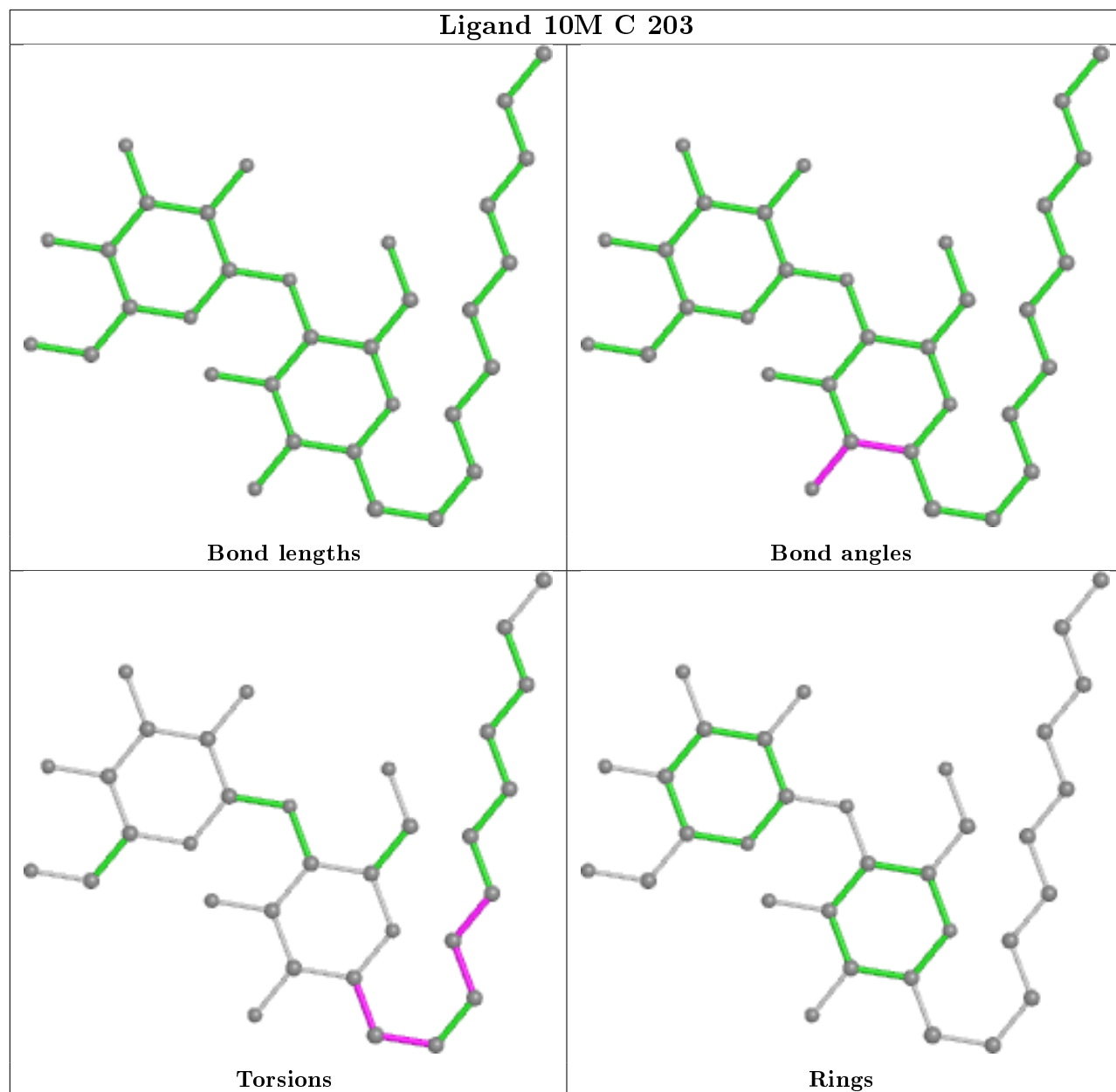
## Ligand HEC A 201





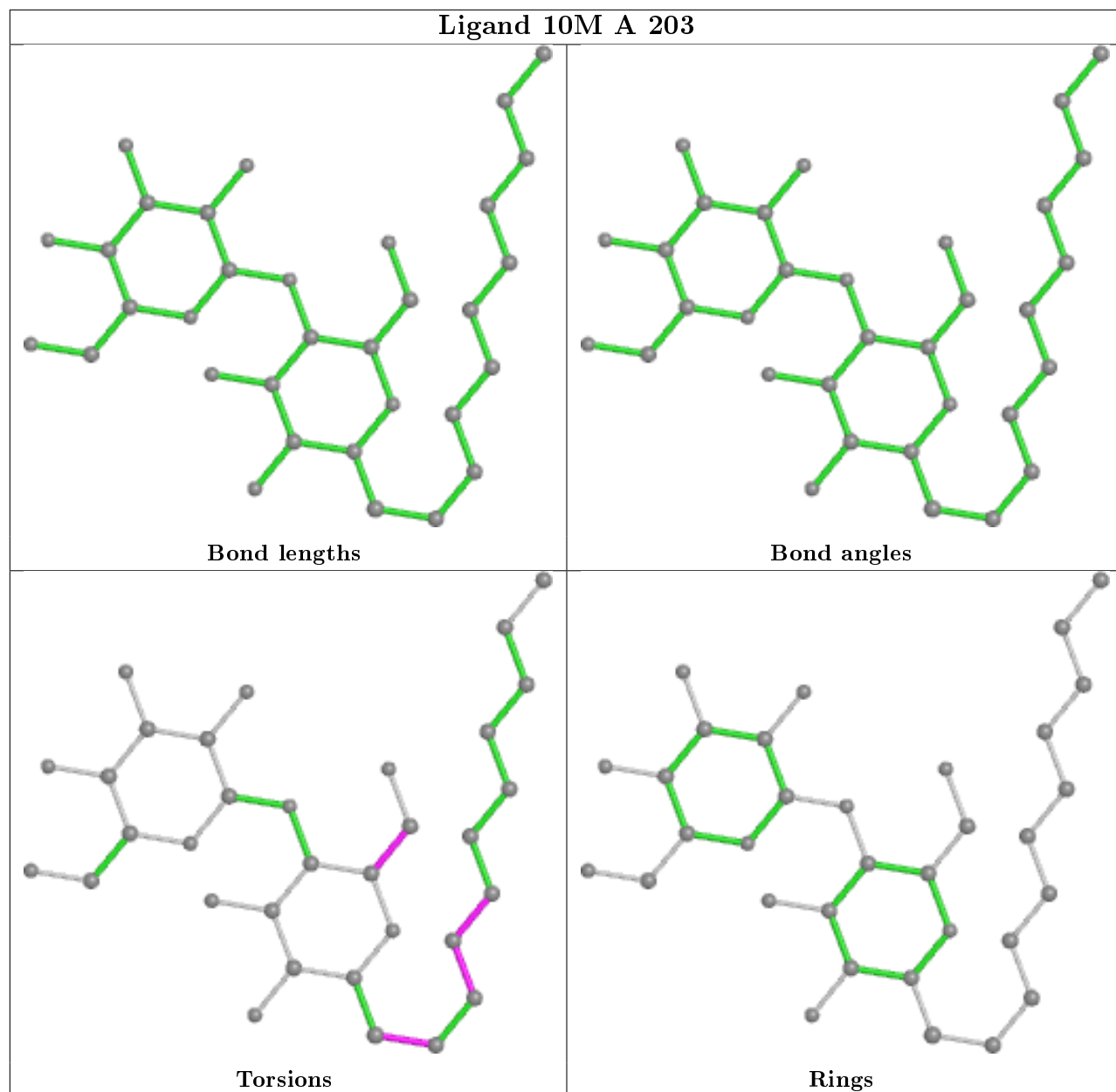


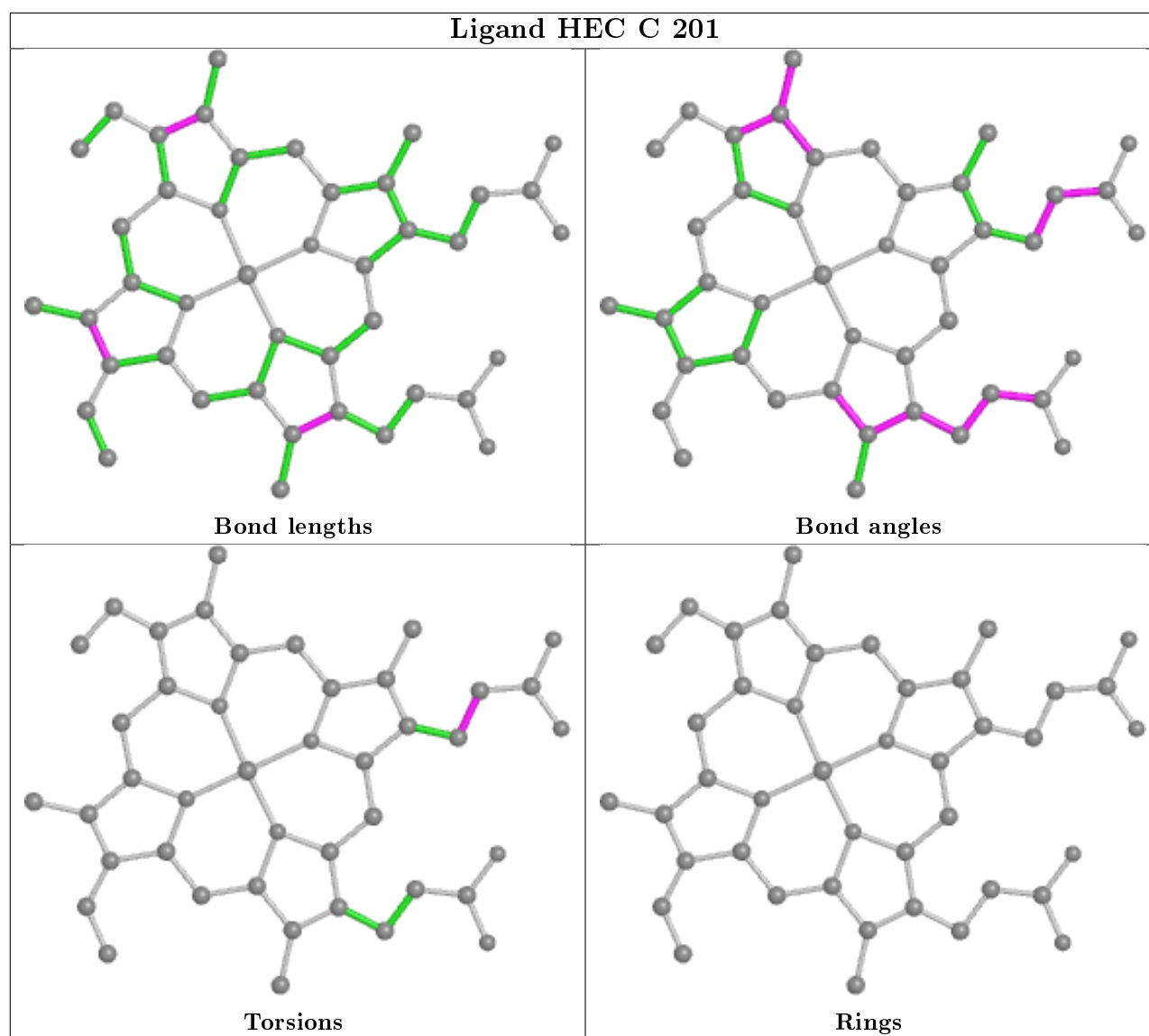
## Ligand 10M C 203





## Ligand 10M A 203





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	142/146 (97%)	-0.20	9 (6%)	20	11	49, 74, 127, 147	0
1	C	142/146 (97%)	-0.44	2 (1%)	75	63	34, 57, 97, 116	0
2	B	449/465 (96%)	-0.41	14 (3%)	49	32	43, 72, 104, 134	0
2	D	449/465 (96%)	-0.47	7 (1%)	72	59	32, 56, 89, 123	0
3	M	538/568 (94%)	-0.52	2 (0%)	92	89	31, 56, 88, 108	0
3	N	538/568 (94%)	-0.29	16 (2%)	50	34	38, 76, 113, 133	0
All	All	2258/2358 (95%)	-0.41	50 (2%)	62	48	31, 65, 105, 147	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	476	GLU	6.9
2	D	373	GLY	6.2
1	A	89	GLU	4.7
2	B	420	ASP	4.6
1	C	88	GLU	4.5
2	D	374	ILE	4.0
1	A	9	MET	3.7
3	M	446	ARG	3.6
1	A	15	PHE	3.6
2	B	422	ALA	3.6
2	D	376	GLU	3.5
1	A	14	TYR	3.3
3	M	144	ASP	3.3
2	B	235	GLU	3.2
2	B	419	ALA	3.1
1	C	89	GLU	3.0
3	N	142	LEU	2.9
2	B	233	ASP	2.8
3	N	421	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
3	N	210	LYS	2.8
2	B	413	TRP	2.8
2	B	128	LEU	2.7
3	N	144	ASP	2.7
1	A	8	GLY	2.7
1	A	5	PHE	2.6
3	N	32	SER	2.6
2	B	421	GLY	2.6
2	D	375	GLY	2.6
3	N	542	VAL	2.5
3	N	408	TYR	2.4
3	N	140	LYS	2.4
1	A	6	THR	2.3
2	B	381	ARG	2.3
3	N	70	GLN	2.3
3	N	145	LEU	2.3
2	D	127	GLU	2.3
2	B	164	ARG	2.2
1	A	88	GLU	2.2
3	N	431	LYS	2.2
2	D	163	LEU	2.2
3	N	407	GLN	2.2
2	B	380	ASN	2.2
3	N	95	GLY	2.2
2	D	372	ARG	2.1
2	B	299	ARG	2.1
1	A	16	GLY	2.1
3	N	138	PRO	2.1
3	N	33	GLU	2.1
2	B	423	ALA	2.0
2	B	417	MET	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

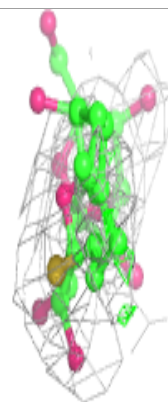
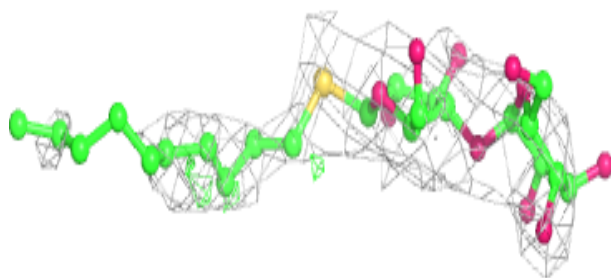
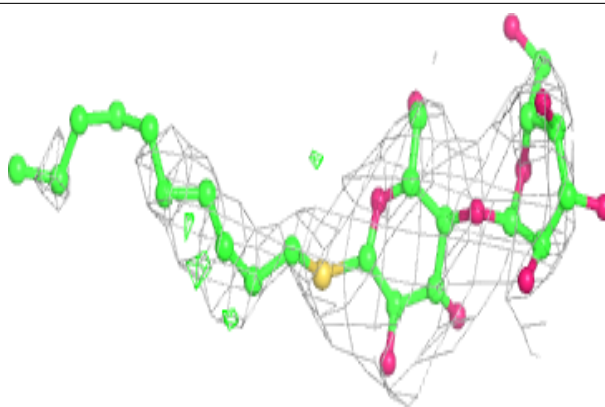
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	10M	D	805	33/33	0.82	0.38	93,114,125,130	0
6	10M	A	203	33/33	0.87	0.39	71,107,122,128	0
6	10M	C	203	33/33	0.90	0.24	71,82,98,110	0
11	CL	N	603	1/1	0.90	0.21	44,44,44,44	0
11	CL	M	603	1/1	0.94	0.34	44,44,44,44	0
10	DHE	N	602	49/49	0.95	0.20	44,53,67,70	0
7	HEM	D	801	43/43	0.97	0.22	37,39,44,46	0
10	DHE	M	602	49/49	0.97	0.18	25,28,34,36	0
4	HEC	N	601	43/43	0.97	0.15	37,42,53,58	0
7	HEM	D	802	43/43	0.97	0.18	41,44,48,51	0
7	HEM	B	801	43/43	0.97	0.18	43,45,53,63	0
4	HEC	A	201	43/43	0.97	0.14	43,46,57,63	0
4	HEC	M	601	43/43	0.98	0.15	31,35,40,42	0
9	O	B	804	1/1	0.98	0.22	33,33,33,33	0
7	HEM	B	802	43/43	0.98	0.17	51,57,70,78	0
5	CA	A	202	1/1	0.98	0.07	32,32,32,32	0
4	HEC	C	201	43/43	0.98	0.15	22,25,32,37	0
8	FE	D	803	1/1	0.99	0.08	19,19,19,19	0
9	O	D	804	1/1	0.99	0.15	11,11,11,11	0
8	FE	B	803	1/1	0.99	0.12	47,47,47,47	0
5	CA	C	202	1/1	0.99	0.12	8,8,8,8	0

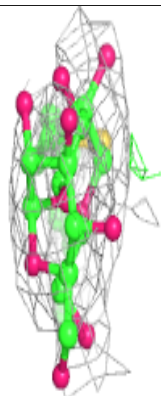
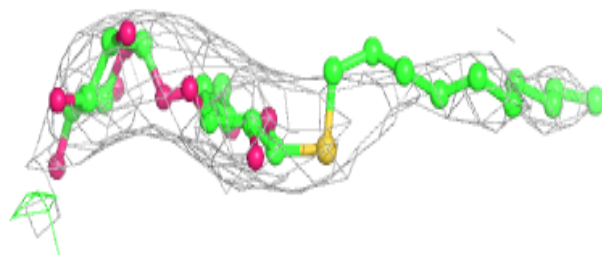
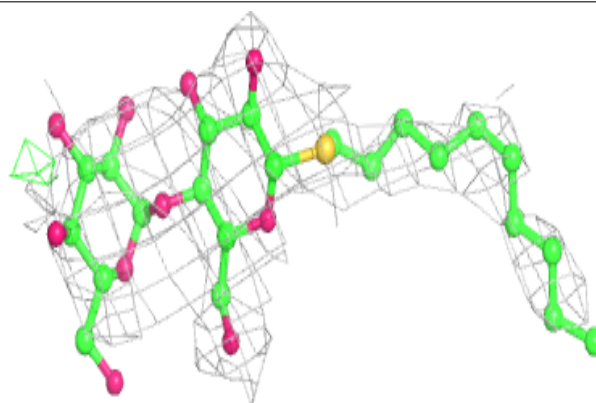
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around 10M D 805:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

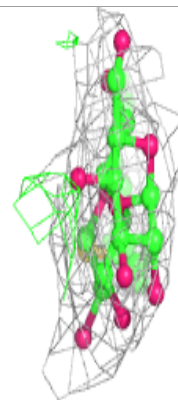
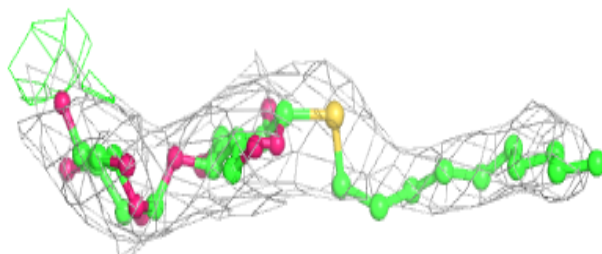
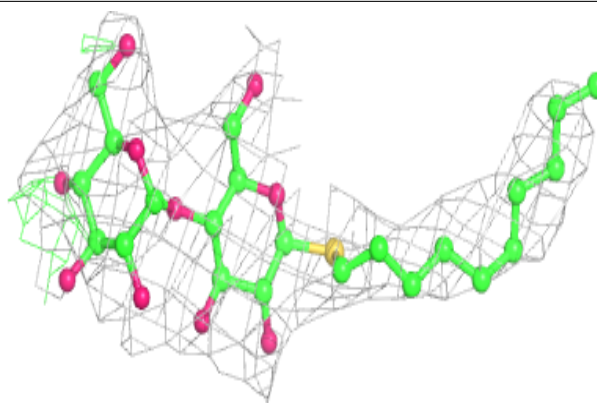
**Electron density around 10M A 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

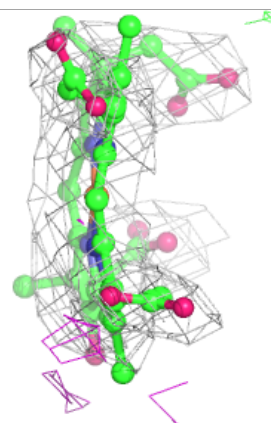
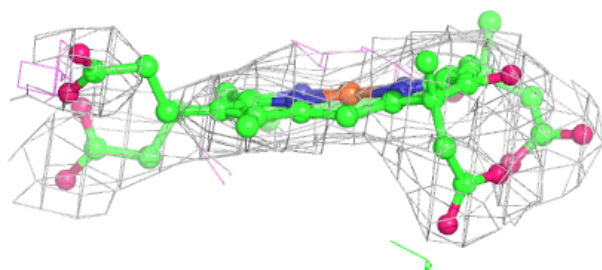
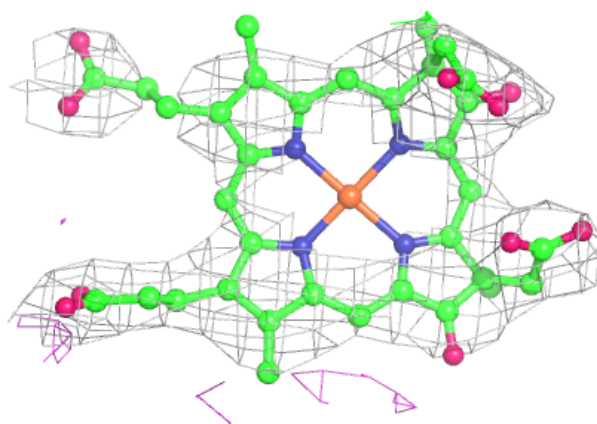


**Electron density around 10M C 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

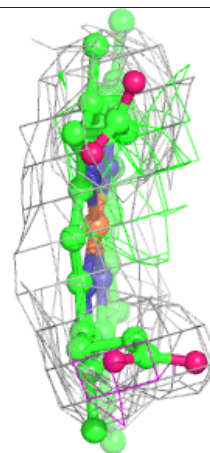
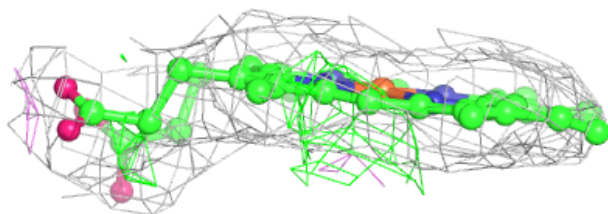
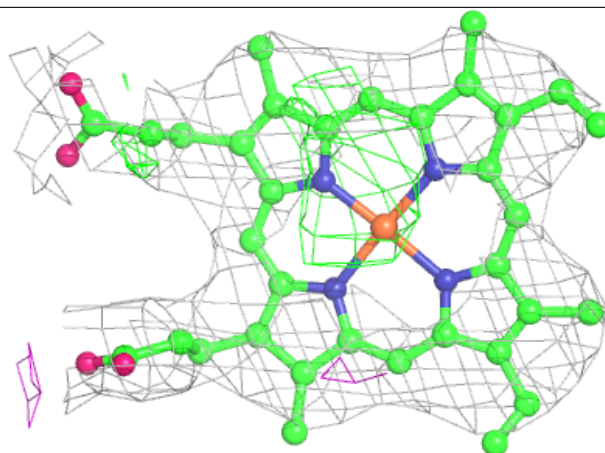
**Electron density around DHE N 602:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM D 801:**

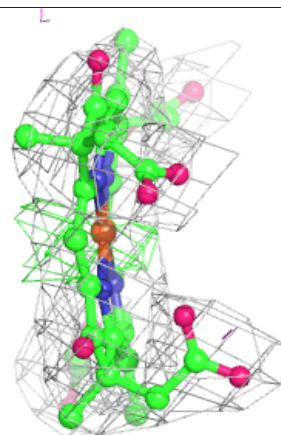
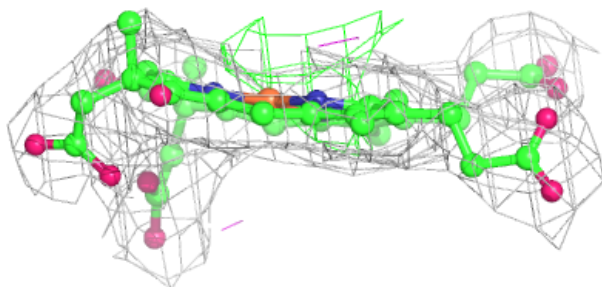
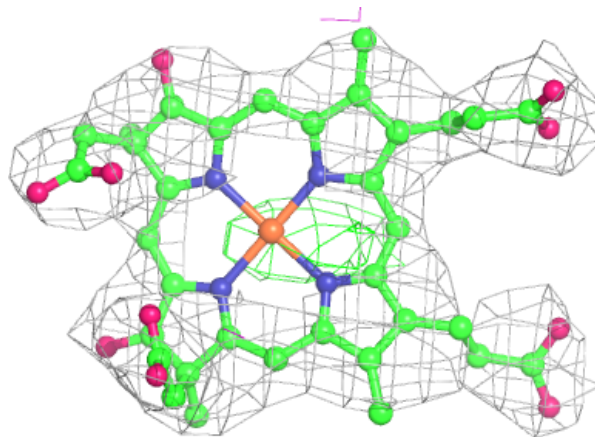
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





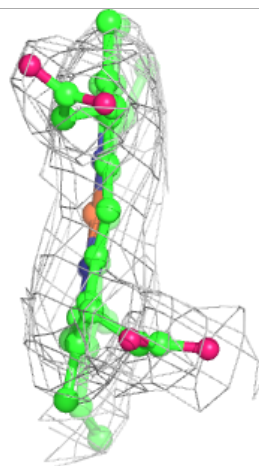
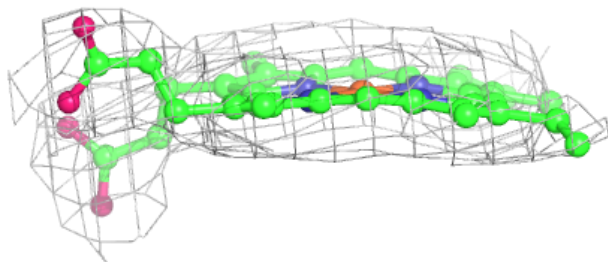
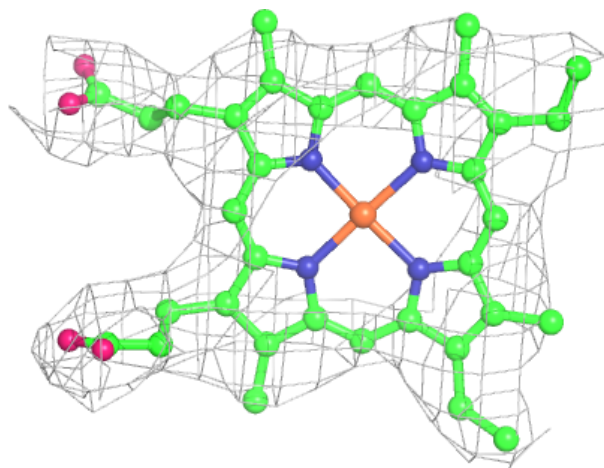
**Electron density around DHE M 602:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



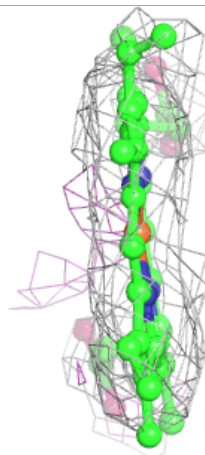
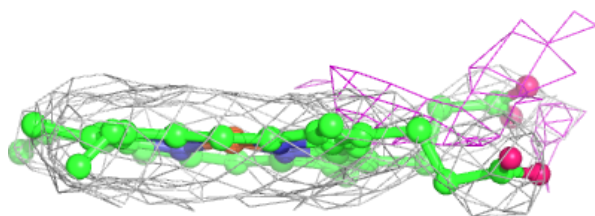
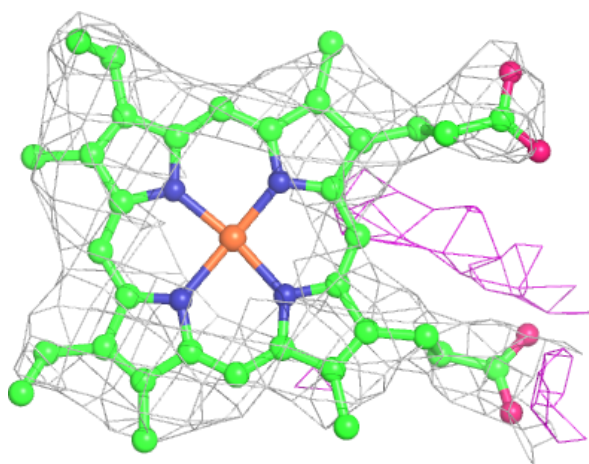
**Electron density around HEC N 601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



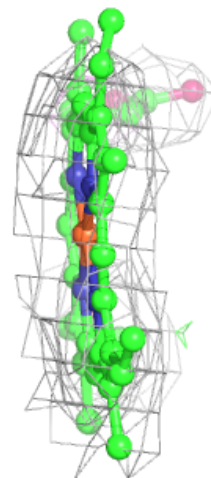
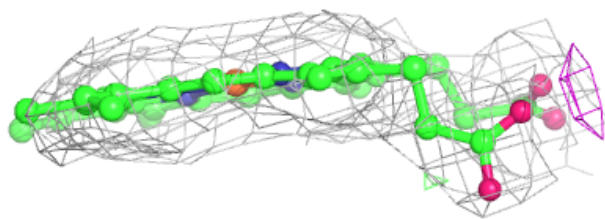
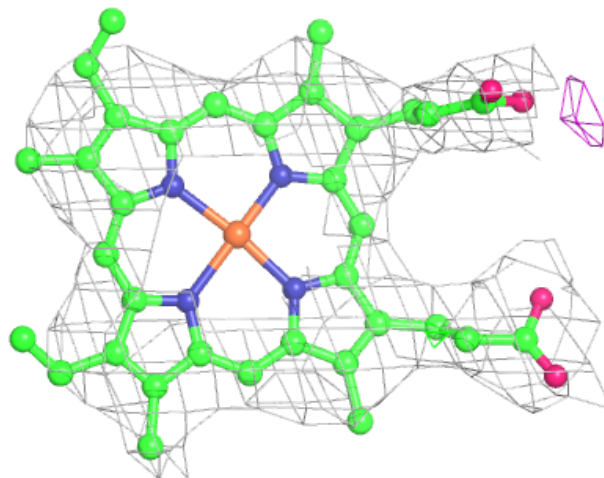
**Electron density around HEM D 802:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



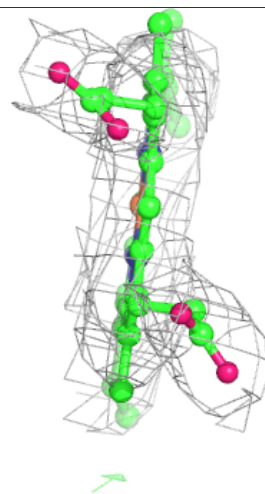
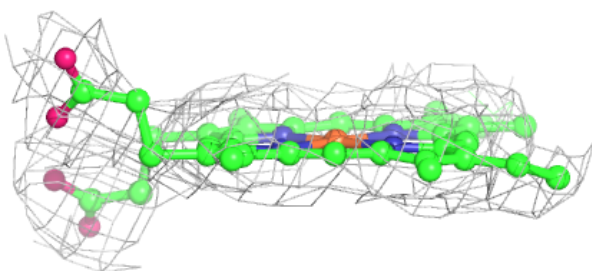
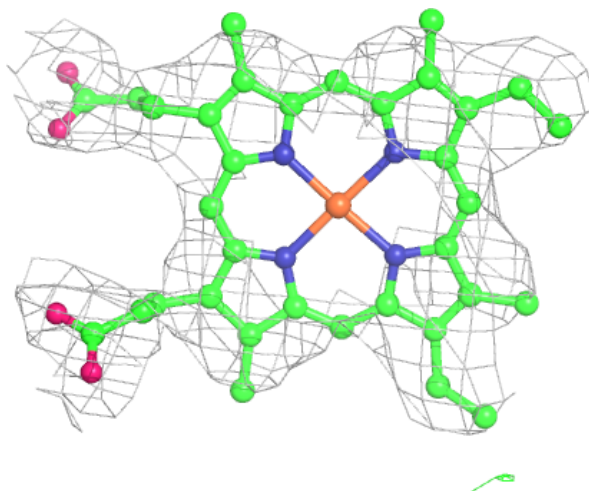
**Electron density around HEM B 801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



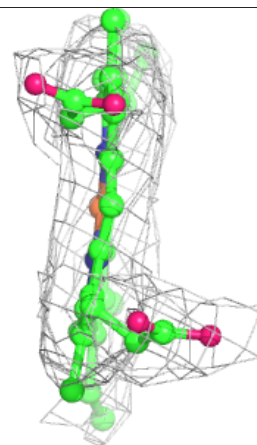
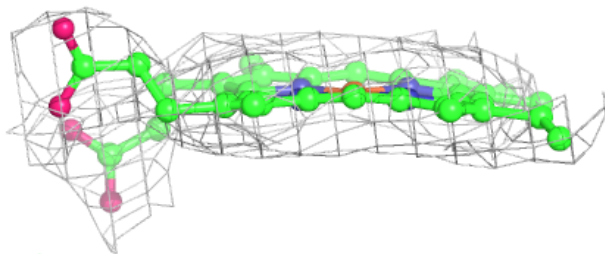
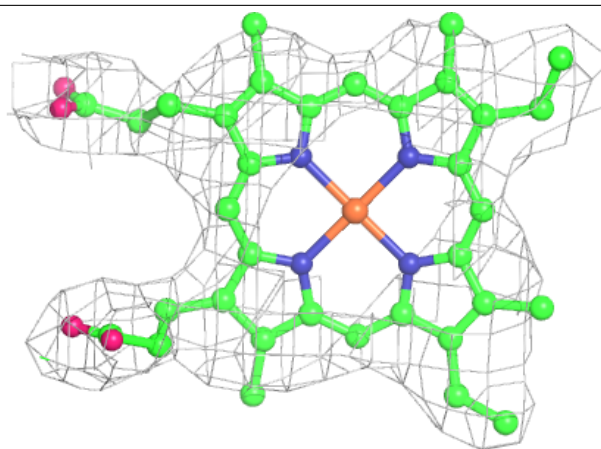
**Electron density around HEC A 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



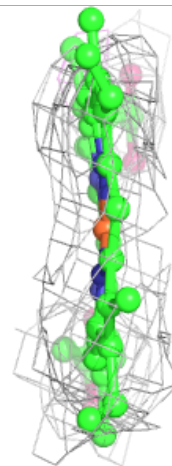
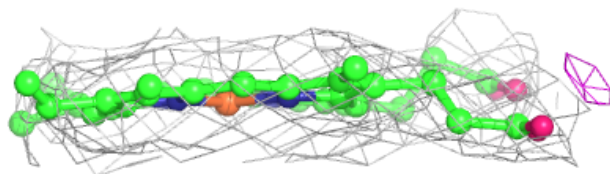
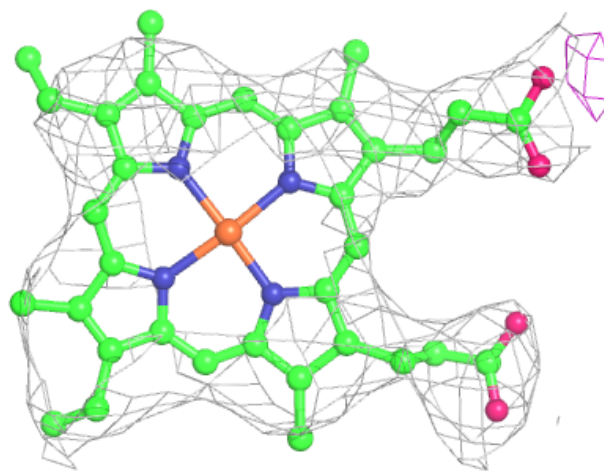
**Electron density around HEC M 601:**

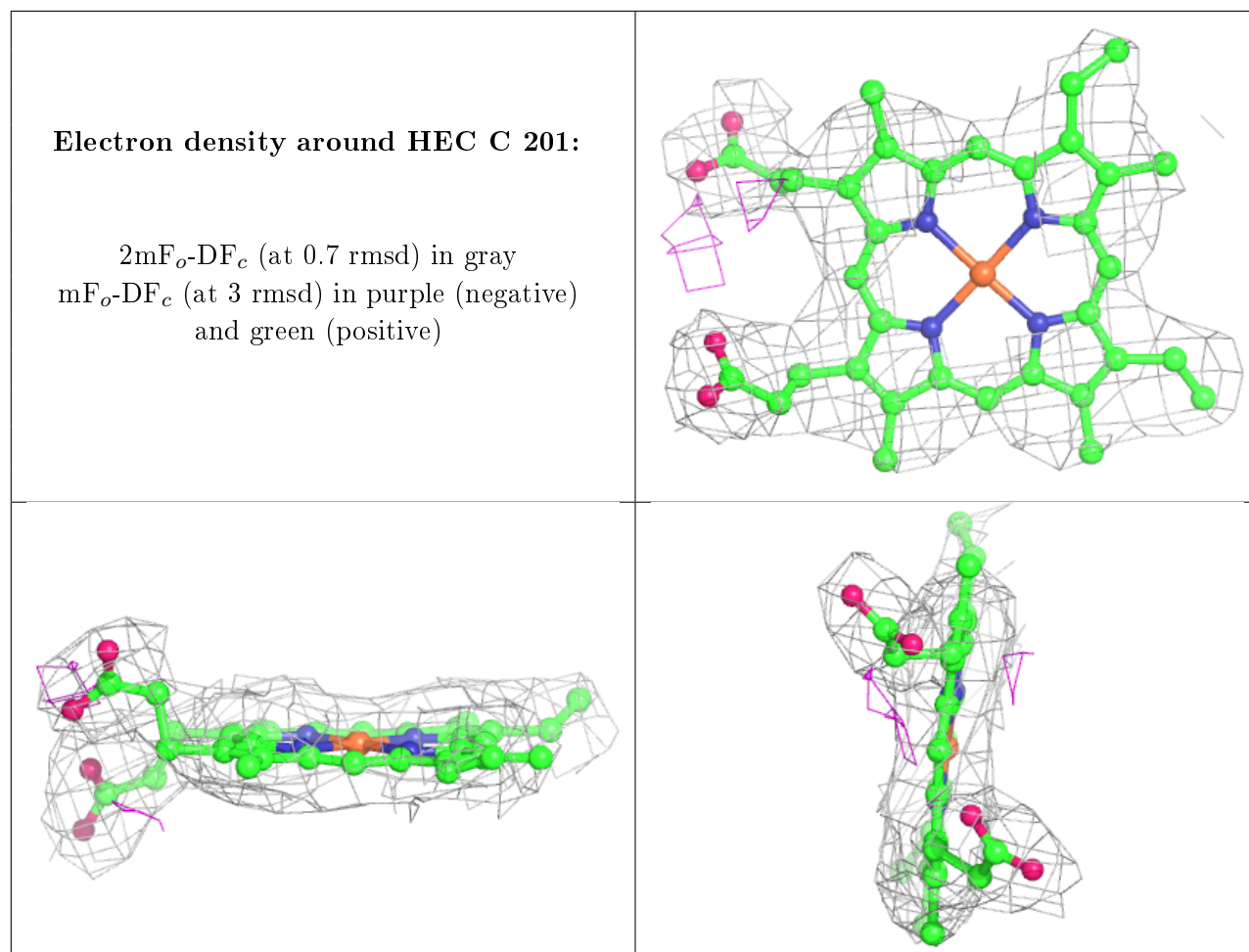
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM B 802:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.